Periodic Hartree-Fock Theory

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Zusammenfassung

Die am häufigsten verwendeten Näherungen an die elektronische Grundzustandsenergie eines quantenmechanischen Modells können schematisch in zwei Hauptklassen eingeteilt werden.

- Dichtefunktionaltheoretische Methoden werden verwendet, um die elektronische Struktur von Vielteilchensystemen zu untersuchen. Sie beruhen auf der Neuformulierung des betrachteten Minimierungsproblems auf die Art und Weise, dass die Hauptvariable die elektronische Dichte ist. Damit eignen sich diese Methoden für Chemiker und Physiker, die an großen molekularen Systemen interessiert sind. Unter Mathematikern ist die Thomas-Fermi-Theorie das prominente Beispiel für ein solches Verfahren. Sie bietet für komplexe Atome mit großen Ordnungszahlen Z, eine nützliche Beschreibung und wurde 1927 als statistisches Modell benutzt, um die Verteilung der Elektronen in einem Atom anzunähern.

- Wellenfunktionsmethoden zielen daraufhin ab, eine Näherung der Grundzustandswellenfunktion und Grundzustandsenergie eines quantenmechanischen Vielteilchensystems zu finden. Die herkömmlichen Ansätze benutzen Wellenfunktionen als zentrale Größe, da sie die vollständigen Informationen eines Systems enthalten. Sie stellen sicher, dass die berechnete Energie von einer geratenen Wellenfunktion eine obere Schranke an die richtige Grundzustandsenergie ist. Eine vollständige Minimierung der Energie in Bezug auf alle erlaubten Wellenfunktionen ergibt also den richtigen Grundzustand. Die Hartree-Fock (HF)-Näherung, die von Hartree eingeführt und von Fock gegen Ende der 1920er Jahre verbessert wurde, ist ein wichtiges Beispiel dieser Methoden. Die HF-Näherung wird von Chemikern benutzt, die sich für genaue Simulationen von kleinen Systemen interessieren, ohne Berücksichtigung der

Zeit der Berechnung.

Diese Näherungsmethoden liefern vereinfachte Beschreibungen der elektronischen Struktur der Atome oder Moleküle. Wir interessieren uns für die zweite Methode, besonders für die periodische HF-Theorie.

Die vorliegende Arbeit umfasst drei Teile: Periodische Minimierer des HF-Funktionals und ihre Eigenschaften, die Blochwellenzerlegung und ihre Anwendung auf die periodische HF-Theorie und die Öffnung einer Lücke im Spektrum einer Faser des HF-Hamiltonoperators, falls es ein schwaches, periodisches, eindimensionales Potential gibt.

Die Übersicht ist wie folgt aufgebaut. In Kapitel 1 wird eine Einführung in die HF-Theorie gegeben und ihre Wichtigkeit als eine Wellenfunktionsmethode zur Näherung der elektronischen Grundzustandsenergie dargestellt. Hier werden die Konzepte der Grundzustandsenergie und der HF-Energie eines Hamiltonoperators auf dem fermionischen Fockraum vorgestellt. Das Energiefunktional wird auf der Menge der normierten antisymmetrischen Produktvektoren definiert, d.h. auf der Menge der Slaterdeterminanten. Sein minimaler Wert wird HF-Energie (E_{hf}) genannt. Die Einschränkung des Variationsraums auf Slaterdeterminanten bietet eine obere Schranke zur Grundzustandsenergie, da die Positionen der Elektronen als unabhängige Variablen betrachtet werden. Um die Differenz $E_{\mathrm{gs}} - E_{\mathrm{hf}}$ zwischen der Grundzustandsenergie und der HF-Energie zu analysieren, ist es zweckmäßig die Einteilchen und die zweiteilchen-Dichtematrizen einzuführen. Sie enthalten Informationen über den Status des Ensembles von Spins zu einem gegebenen Zeitpunkt. Dieser Formalismus stellt die Quantenzustände in einer einfacheren Form dar. Der Ausdruck der HF-Energie in Bezug auf Dichtematrizen ist mathematisch unvorteilhaft, da die Slaterdeterminanten, die die Dichtematrizen erzeugen, keine lineare Struktur haben. Allerdings bestätigt das Liebsche Variationsprinzip (Theorm 1.1), dass die Variation über N Projektionen (d.h. über Dichtematrizen, die von Slaterdeterminanten erzeugt werden) das gleiche Ergebnis liefert wie die Variation über alle, zu irgendwelche N Fermionen-Zustände gehörende Einteilchendichtematrizen. In Abschnitt 1.1.1 geben wir einige für unsere Arbeit wichtige Ergebnisse von Lieb und Solovej über die Existenz eines HF-Minimierers. Der Rest von Kapitel 1 konzentriert sich auf die periodische HF-Theorie, wo das periodische Modell und das entsprechende Variationsproblem in 1.2 bzw. 1.2.1 eingeführt werden.

Kapitel 2 ist der Untersuchung der Eigenschaften der periodischen HF-Minimierer gewidmet. In Theorem 2.2 wird die Existenz eines periodischen HF-Minimierers mit

Argumenten, die ähnlich zu denen von Catto, Le Bris und Lions in [14] sind, ausgeführt. Die grundlegende Strategie in diesem Beweis besteht darin, dass ein Netz $\{\gamma_n\}_{n\in I}$ [1] von Dichtematrizen in der Variationsmenge der periodischen Minimierer $P_{\text{per}}^{(N)}$ betrachtet wird, so dass das HF-Funktional $\mathcal{E}_{hf}(\gamma_n)$ gegen die periodischen HF-Grundzustandsenegie $E_{hf}^{\text{per}}(N)$ konvergiert. Dann wird bewiesen, dass dieses Netz γ_n bis auf eine Teilnetz gegen einen Operator $\gamma \in P_{\text{per}}^{(N)}$ mit $\mathcal{E}_{hf}(\gamma) = E_{hf}^{\text{per}}(N)$ konvergiert. Letzteres wird durch die Konstruktion einer schwach* Topologie auf $P_{\text{per}}^{(N)}$ und anschließender Anwendung von Arazy's Theorem [27], für den Übergang zur starken Konvergenz gezeigt. Außerdem wird in Theorem 2.3 verifiziert, dass ein periodischer Minimierer eine Projektion auf die N niedrigsten Eigenwerte des HF-Hamiltonoperators ist. Der vorgestellte Beweis ist eine Adaption des Beweises von Bach, Fröhlich and Jonson in [33] mit der Einschränkung auf den periodischen Fall. Ferner wird in Lemma 2.5 durch Widerspruch zur Minimalität des periodischen Minimierers bewiesen, dass eine Lücke im Spektrum des HF-Hamiltonoperators oberhalb des N-ten Energieniveaus existiert. Darüber hinaus wird die Eindeutigkeit des Minimierers auf $P_{\text{per}}^{(N)}$ in Theorem 2.4 durch Anwendung einer selbstkonsistenten Gleichung und des Banachschen Fixpunktsatzes gezeigt. Dieser Beweis orientiert sich an der Arbeit von Griesemer und Hantsch [11], die auf dem Artikel von Huber und Siedentop über die Lösungen der Dirac-Fock-Gleichungen basiert. In diesem Zusammenhang ist die Annahme wesentlich, dass der N-te Eigenwert des freien Hamiltonoperators durch eine Lücke von seinem restlichen Spektrum getrennt ist. Die Existenz einer solchen Lücke zeigt, dass die Energie sich bei dem Übergang von dem periodischen Minimierer auf die Menge der nicht periodischen Matrizen erhöht. Dies bedeutet, dass die HF-Energie und die periodische HF-Energie bei dem periodischen Minimierer übereinstimmen.

In Kapitel 3 werden die periodischen Eigenschaften des HF-Minimierers auf $\mathfrak{H}_\Lambda = L^2(\Lambda)$ für einen gegebenen Torus $\Lambda := \mathbb{R}^d/(L\mathbb{Z})^d$ untersucht. Ein Einheitswürfel $Q := \Lambda/\Gamma$ und ein Gitter $\Gamma := (q\mathbb{Z})^d/(L\mathbb{Z})^d$ von Λ werden definiert, um $\mathfrak{H}_\Lambda$ gemäß der Translationsinvarianz aus Vektoren von Γ zu zerlegen. Aus dieser Zerlegung von Funktionen in $\mathfrak{H}_\Lambda$ in Blochwellen kann eine direkte Zerlegung von Operatoren K auf $\mathfrak{H}_\Lambda$ abgeleitet werden. Dies gilt in dem Sinne, dass die spektrale Analyse von K auf

[1] I bezeichnet eine gerichtete Menge, d.h., eine nichtleere Menge I versehen mit einer Relation $<$ über I (genannt Richtung), die folgenden Axiomen genügt:

(i) Falls $\alpha, \beta \in I$ sind, dann existiert $\gamma \in I$, so dass $\gamma > \alpha$, $\gamma > \beta$ sind.

(ii) $<$ ist eine Halbordnung.

die spektrale Analyse der Familie seiner Fasern reduziert wird. Durch Anwendung dieser Konstruktion auf die periodischen Dichtematrizen ergeben sich entsprechende Aussagen für ihre Periodizität (Lemmas 3.1 and 3.3). Außerdem ist eine Version des Satzes von Bloch in Lemma 3.5 wiedergegeben. Diese besagt, dass jeder Eigenvektor eines Hamiltonoperators mit periodischem Potential in Form einer Wellenfunktion gewählt werden kann. Diese Wellenfunktion ist die Multiplikation von einer Funktion, die die gleiche Periodizität wie das Potential hat, mit der komplexen Phase einer ebenen Welle, die den Betrag eins hat.

Kapitel 4 beschäftigt sich mit der Charakterisierung des periodischen HF-Minimierers. Die Fasern des periodischen Hamiltonoperators und des HF Funktionals werden explizit in Lemmata 4.1 and 4.3 berechnet. Ihre Aussagen werden in dem verallgemeinerten Beweis von Theorem 5.1 über das Liebsche Variationsprinzip im periodischen Fall verwendet. Mit Hilfe der Beweiskonstruktion kann eine Abschätzung der Differenz zwischen dem $N+1$-ten und dem N-ten Eigenwert einer Faser des Hamiltonoperators in Bezug auf die entsprechende Faser des periodischen Potentials gegeben werden.

Im letzten Kapitel wird ein neues Modell untersucht. Wir betrachten den Hilbertraum $\mathfrak{H}_\Lambda = \ell^2(\Lambda)$ mit einem diskreten Torus $\Lambda := \mathbb{Z}^d/(L\mathbb{Z})^d$. Der Hamiltonoperator des Systems besteht aus dem diskreten Laplaceoperator sowie einem Wechselwirkungspotential, das mit einem Multiplikationsoperator mit einer positiven, symmetrischen Funktion $W : \Lambda \longrightarrow \mathbb{R}_+$ identifiziert wird. Im Eindimensionalen wird der diskrete Laplaceoperator direkt mit Hilfe der definierten Blochwellenzerlegung von Elementen in $\mathfrak{H}_\Lambda$ diagonalisiert. Darüber hinaus ist die Diagonalmatrix einer Faser des HF-Hamiltonoperator explizit berechenbar, was in Lemma 5.3 gezeigt wird. Schließlich wird in Lemma 5.4 bewiesen, dass der Abstand zwischen den nebeneinanderliegenden Eigenwerten einer Faser des HF-Hamiltonoperators steigt, falls ein periodisches schwaches Potential mit beschränktem Träger existiert.

Summary

The most commonly used approximations to the electronic ground state energy of a quantum mechanical model can schematically be classified into two main classes:

- Density functional methods are used to investigate the electronic structure of many-body systems. They are based on reformulation of the considered minimization problem in such a way that the main variable is the electronic density. This makes these methods efficient for chemists and physicists who are interested in large molecular systems. The Thomas-Fermi model is considered as the prominent example of such a method among mathematicians. It provides for complex atoms with large atomic number Z, a useful description and used as a statistical model in 1927 to approximate the distribution of the electrons in an atom.

- Wave function methods aim at finding an approximation of the ground state wave function and the ground state energy of a quantum many-body system. The conventional wave function approaches use wave function as the central quantity, since it contains the full information of a system. They assure that the energy computed from a guessed wave function is an upper bound to the true ground state energy. Full minimization of the energy with respect to all allowed wave functions will give the true ground state. The Hartree-Fock approximation, introduced by Hartree and improved by Fock in the late 1920s, is an important example of these methods. It is widely used by chemists who are interested in the precise simulations of small systems without considering the time of computation.

These approximation methods give a simplified quantum description of the electronic structure around the nuclei. We are interested in the second method, especially in the

periodic Hartree-Fock theory. The present thesis includes three parts, the periodic minimizer of the Hartree-Fock (HF) functional and its properties, the Bloch wave decomposition and its application on the periodic HF theory and the opening gap in the spectrum of the fibered HF Hamiltonian in the presence of a weak, periodic one-dimensional potential.

The overview is organized as follows. In Chapter 1 an introduction to HF theory and its importance as a wave function method for finding an approximation of the electronic ground state energy is provided. Here the concepts of the ground state energy and the HF energy of a Hamiltonian acting on the fermion Fock space are presented. The energy functional is defined on the set of normalized antisymmetric product vectors, i.e., on the set of Slater determinants. Its minimal value is called HF energy (E_{hf}). The restriction of the variational space in the variational problem to Slater determinants provides that the HF energy is an upper bound of the ground state energy. To study the difference $E_{gs} - E_{hf}$ it is convenient to introduce one-particle (1-pdm) and two-particles (2-pdm) density matrices, since they contain information about the status of the ensemble of spins at a given time and their formalism represent the quantum states in a simpler way. The HF energy of density matrices induced by some Slater determinants is mathematically inconvenient due to the lack of linear structure of the set of Slater determinants. But Lieb's variational principle (Theorem 1.1) asserts that the variation over rank N projections (i.e., over the one periodic density matrices induced by some Slater determinants) gives the same result as the variation over all 1-pdm that belong to any N fermion states. For the readers convenience in Subsection 1.1.1 some results are recalled without proofs due to Lieb and Solovej concerning the existence of the HF minimizer. The rest of Chapter 1 focuses on the periodic HF theory, where the periodic model and the corresponding variational problem are introduced in sections 1.2 and 1.2.1, respectively.

Chapter 2 is devoted to the study of the properties of the periodic HF minimizer. In Theorem 2.2, the existence of the periodic HF minimizer using arguments similar to those of Catto, Le Bris and Lions in [14] will be achieved. The basic strategy in this proof is to consider a net $\left\{\gamma_n\right\}_{n\in I}$ [2] of density matrices in the variational set of periodic minimizers $P^{(N)}_{\mathrm{per}}$ such that the HF functional $\mathcal{E}_{hf}(\gamma_n)$ tends to the periodic

[2] I denotes a directed system, i.e., an index set together with an ordering $<$ which satisfies:

(i) If $\alpha, \beta \in I$, then there exists $\gamma \in I$ so that $\gamma > \alpha$, $\gamma > \beta$.

(ii) $<$ is a partial ordering.

ground state energy $E_{hf}^{\text{per}}(N)$ as n tends to infinity. Then it will be proved that this net converges, up to the extraction of a subnet, to some operators $\gamma \in P_{\text{per}}^{(N)}$ satisfying $\mathcal{E}_{hf}(\gamma) = E_{hf}^{\text{per}}(N)$. The latter can be seen by constructing a weak* topology on $P_{\text{per}}^{(N)}$ and applying Arazy's theorem [27] to obtain strong convergence. Moreover, the fact that the periodic minimizer is a projection onto the N lowest eigenvalues of the periodic HF Hamiltonian is verified in Theorem 2.3. The presented proof is an adaptation of the one given by Bach, Fröhlich and Jonsson in [33], restricted to the periodic case. Furthermore, in Lemma 2.5 it is proven by contradiction to the minimality of the periodic minimizer that there is a gap in the spectrum of the periodic HF Hamiltonian above the N-th energy level. In addition, the uniqueness of the minimizer on $P_{\text{per}}^{(N)}$ is shown in Theorem 2.4 by using the self-consistent equation it satisfies and the contraction mapping principle as in the the work of Griesemer and Hantsch [11], which was based on the paper of Huber and Siedentop on solutions of the Dirac-Fock equations [13]. Here the assumption that the N-th eigenvalue of h is separated by a gap of a positive size from the rest of the spectrum is essential. The presence of such a gap implies that the energy increases by moving from the periodic minimizer even in the set of non periodic matrices, which means that the HF and the periodic HF functional coincide at the periodic minimizer.

In Chapter 3 the periodic properties of the HF minimizer on $\mathfrak{H}_\Lambda = L^2(\Lambda)$ for a given torus $\Lambda = \left(\mathbb{R}^d/(L\mathbb{Z})^d\right)$ is studied. A unit cube $Q = \Lambda/\Gamma$ and a lattice $\Gamma = (q\mathbb{Z})^d/(L\mathbb{Z})^d$ of Λ are introduced to decompose $\mathfrak{H}_\Lambda$ according to the translational invariance by vectors of Γ. After this decomposition of functions in $\mathfrak{H}_\Lambda$ into Bloch waves a direct integral decomposition of operators K on $\mathfrak{H}_\Lambda$ can be derived, in the sense that the spectral analysis of K reduces to the spectral analysis of its fibers. Applying this construction to the periodic density matrices yields an equivalent statement for their periodicity (Lemmas 3.1 and 3.3). Moreover, a version of Bloch's theorem adapted to our framework is given in Lemma 3.5. It states that every eigenvector of a Hamiltonian with periodic potential can be chosen in the form of a wave function, which is a multiplication of a function having the same periodicity as the potential with the complex phase of a plane wave of absolute value one (Bloch's theorem).

Chapter 4 is dedicated to the characterization of the periodic HF minimizers. The fibers of the periodic HF Hamiltonian and that of the periodic HF functional are explicitly computed in Lemmas 4.1 and 4.2, respectively. Theses expressions are used to generalize Lieb's variational principle in the periodic case in Theorem 4.1. By using this proof, an estimate on the distance between the $N+1$-th and the N-

th eigenvalue of the fibered Hamiltonian is obtained in terms of the corresponding fibered periodic potential.

In the last chapter another model is studied. The Hilbert space of states is given by $\mathfrak{H}_\Lambda = \ell^2(\Lambda)$ where $\Lambda = \mathbb{Z}^d/(L\mathbb{Z})^d$ is a discrete torus and the Hamiltonian consists of the discrete Laplace operator plus an interaction which is identified with a multiplication operator with a positive symmetric function $W : \Lambda \longrightarrow \mathbb{R}_+$. In dimension $d = 1$ we show that the discrete Laplace operator can be diagonalized directly via the Bloch wave decomposition defined on $\mathfrak{H}_\Lambda$. Moreover, the diagonal matrix of the fibered Hamiltonian is explicitly computed in Lemma 5.2. Finally, it is shown in Lemma 5.3 that if the support of the periodic potential is bounded then the distance between the consecutive eigenvalues of the fibered Hamiltonian increases in the presence of a weak, positive periodic potential.

Contents

Chapter 1

Hartree-Fock Theory

Contents

Summary

The Hartree-Fock (HF) approximation is one of the most important approximation methods in quantum mechanics of many particles. It is assumed that each electron's motion can be described by a single particle function which does not depend explicitly on the instantaneous motion of other electrons. This simplification causes a loss of correlation between the electrons and hence induces some errors in the result obtained. This chapter is based on the papers [1, 2, 7, 16, 19, 28]. In Section 1.1 is illustrated that the HF theory consists of restricting the variational space $\mathcal{H}$ in the variational problem (1.4) to that of functions of variables $(x_1, \ldots, x_N) \in \mathbb{R}^{dN}$ which can be written as a single determinant (i.e., an antisymmetrized product) of N functions of one variable. This determinant is named for its discoverer, John C. Slater, who proposed Slater determinants as a mean of ensuring the antisymmetry of wave functions through the use of matrices. The Slater determinants of N orbitals define subset of the Hilbert space of all N fermion wave functions without linear structure. This implies that the expression of the HF functional in terms of the one-particle

density matrix (1-pdm)[1] obtained from a Slater determinant is mathematically inconvenient. Lieb's important observation given in Lemma 1.1 solves this problem by relaxing the condition on the 1-pdm without changing the infimum. The next section is devoted to the study of the existence of the HF minimizer. For the readers convenience some results due to Lieb, Solovej, Enstedt and Melgaard are recalled without proof which give the conditions for the existence of such a minimizer. In the last section the periodic HF model is defined in 1.2, where a unit cube Q and a lattice Γ of a given torus are considered to specify the periodic variational problem (1.17).

1.1 Hartree-Fock Theory

In the HF theory, in contrast to the Schrödinger theory, the total N-particle Hilbert space

$$\mathcal{H} = \bigwedge^{N} \mathfrak{H},$$

is not considered, with $\mathfrak{H} := L^2(\mathbb{R}^d; \mathbb{C}^2)$. The attention is rather restricted to the Slater determinants:

$$\begin{aligned}\Phi : &= (N!)^{-\frac{1}{2}}\, \varphi_1 \wedge \ldots \wedge \varphi_N \\ &= \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(x_1) & \ldots & \varphi_1(x_N) \\ . & \ldots & . \\ . & \ldots & . \\ . & \ldots & . \\ \varphi_N(x_1) & \ldots & \varphi_N(x_N) \end{vmatrix}. \end{aligned} \tag{1.1}$$

with $\varphi_1, \ldots, \varphi_N \subseteq \mathfrak{H}$ being an orthonormal subset of $\mathfrak{H}$, $\langle \varphi_i \mid \varphi_j \rangle = \delta_{i,j}$. The set of all $\Phi \in \mathcal{H}$ is called the set of Slater determinants and denoted by $\mathcal{SD}_N$. The HF approximation consists of restricting the variational space $\mathcal{H}$ in the variational problem to that of functions of the variables $(x_1, \ldots, x_N) \in \mathbb{R}^{dN}$ that can be written as an antisymmetrized product of N functions defined on $\mathbb{R}^d$. Then the energy expectation value

$$\frac{\langle \Phi | H_N \Phi \rangle}{\langle \Phi | \Phi \rangle}, \tag{1.2}$$

[1] see for more details Appendix A

is minimized over all wave functions of the form (1.1), where in units such as $\frac{\hbar^2}{2m} = 1 = |e|$, the N-electron Hamiltonian H_N in (1.2), e.g., for an atom, is given by

$$\begin{aligned} H_N(\underline{Z}, \underline{R}) &:= \sum_{i=1}^{N} \left(-\Delta_i - Z\, |x_i|^{-1} \right) + \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} \\ &:= \sum_{i=1}^{N} h_i + \sum_{1 \le i < j \le N} W_{i,j}, \end{aligned} \tag{1.3}$$

acting as a self-adjoint operator on a dense domain $D_N \subseteq \mathcal{H}$ of antisymmetric spinor-valued functions. Above the nucleus of charge Z is regarded as a point charge at the origin surrounded by N electrons of spin $\frac{1}{2}$ and $(x_1, \ldots, x_N) \in \mathbb{R}^{dN}$ with $x_n = \left(x_n^{(1)}, \ldots, x_n^{(d)} \right) \in \mathbb{R}^d$ being the position of the n-th electron. The HF approximation is based on a mean field approximation in that each electron is only subject to the average influence of the other electrons. This simplification causes a loss of correlation between the electrons which leads to some errors in the result obtained. Therefore, restricting the minimization problem to functions of the form (1.1) gives an upper bound of the exact energy which is a virtue of this method in comparison to other approximation methods. Now the HF approximation is introduced in a more explicit fashion. In this process density matrices are used, which are presented in a concise form in Appendix A, as well as a fixed particle sector $\mathcal{H}$ [2] to which we may restrict without loss of generality, since the Hamiltonian H_N commutes with the number operator $\mathcal{N}$.

Definition 1.1. *1. The ground state energy $E_{\mathrm{gs}}(N)$ of H_N for a fixed particle number $N \in \mathbb{N}$ is defined by:*

$$E_{\mathrm{gs}}(N) := \inf \left\{ \langle \Phi | H_N \Phi \rangle \;\middle|\; \Phi \in \mathcal{H},\ \|\Phi\|_{\mathcal{H}} = 1,\ \mathcal{N}\Phi = N\Phi \right\}. \tag{1.4}$$

2. For $\gamma \in \mathscr{L}^1(\mathfrak{H})$ [3], $\gamma = \gamma^* = \gamma^2$, $\mathrm{Tr}_{\mathfrak{H}}(\gamma) = N, \mathrm{Tr}_{\mathfrak{H}}\{h\,\gamma\} < \infty$, where h is the one-particle operator on $\mathfrak{H}$, the HF functional is given by

$$\mathcal{E}_{\mathrm{hf}}(\gamma) \;:=\; \mathrm{Tr}_{\mathfrak{H}}\{h\,\gamma\} \;+\; \frac{1}{2}\,\mathrm{Tr}_{\mathfrak{H}\otimes\mathfrak{H}}\Big\{ V\,(1 - \mathrm{Ex})\,(\gamma \otimes \gamma) \Big\}, \tag{1.5}$$

where $\mathrm{Ex} : f \otimes g \longmapsto g \otimes f$ is the exchange operator on $\mathfrak{H} \otimes \mathfrak{H}$.

[2] $\mathcal{H}$ denotes the antisymmetric subspace of $\bigotimes_N \mathfrak{H}$.

[3] $\mathscr{L}^1(\mathfrak{H})$ denotes the space of trace-class operators on $\mathfrak{H}$.

3. *The HF energy $E_{hf}(N)$ for $N \in \mathbb{N}$ particles is defined by*

$$\begin{aligned} E_{hf}(N) &:= \inf\left\{\langle\Phi \mid H_N\Phi\rangle \mid \Phi \in \mathcal{SD}_N,\ \langle\varphi_i \mid \varphi_j\rangle = \delta_{ij}\right\} \\ &= \inf\left\{\mathcal{E}_{hf}(\gamma) \mid \gamma = \gamma^* = \gamma^2,\ \mathrm{Tr}_{\mathfrak{H}}(\gamma) = N,\ \mathrm{Tr}_{\mathfrak{H}}\{h\,\gamma\} < \infty\right\}, \end{aligned} \tag{1.6}$$

where the proof of the second equation can be found in Appendix A. A vector Φ_{hf} of the form (1.1) *with the property*

$$E_{\mathrm{hf}}(N) = \langle\Phi_{\mathrm{hf}}|H_N\Phi_{\mathrm{hf}}\rangle, \tag{1.7}$$

is called a HF state of H_N. The corresponding 1-pdm γ_Φ is called a HF state, as well.

If a minimizer γ_0 exists it can be said that the system has a HF ground state described by γ_0. In particular its density is denoted by $\rho_{\gamma_0}(x)$, where

$$\rho_{\gamma_0}(x) = \gamma_0(x, x) \tag{1.8}$$

can be defined explicitly [see Eq.(1.12)]. The set of Slater determinants does not have a linear structure, therefore the expression of the HF energy in (1.6) is mathematically inconvenient. Lieb's important observation was that the infimum of the HF functional is not lowered by extending the functional over all density matrices (over all 1-pdm which can be defined not only for Slater determinants but for any many-particle wave function and even for any mixed state with particle number expectation value N), i.e., the condition that γ is induced by some Slater determinant Φ can be dropped.

Theorem 1.1 (Lieb's Variational principle)**.** *For all $N \in \mathbb{N}$ applies*

$$\begin{aligned} &\inf\left\{\mathcal{E}_{\mathrm{hf}}(\gamma)\,\middle|\,\gamma = \gamma^* = \gamma^2,\ \mathrm{Tr}_{\mathfrak{H}}(\gamma) = N,\ \mathrm{Tr}_{\mathfrak{H}}\{h\,\gamma\} < \infty\right\} \\ &\quad = \inf\left\{\mathcal{E}_{\mathrm{hf}}(\gamma)\,\middle|\,0 \le \gamma \le \mathbb{1},\ \mathrm{Tr}_{\mathfrak{H}}(\gamma) = N,\ \mathrm{Tr}_{\mathfrak{H}}\{h\,\gamma\} < \infty\right\} \end{aligned}$$

and if the infimum over all density matrices is attained, then so is the infimum over projections.

The proof of this theorem is simplified by Bach in [1].

1.1.1 Existence of HF Minimizers and their Properties

From equation (1.4) we note that there always exists an $\varepsilon-$approximative pure ground state, i.e., for every $\varepsilon > 0$ an N-particle state Φ exists, such that $\langle\Phi|H_N\Phi\rangle \le$

$E_{gs}(N) + \varepsilon$. In view of its importance for computational issues, the mathematical difficulties are first outlined by verifying the existence of such a minimizer. Roughly speaking, problem (1.6) is set in the whole space $\mathbb{R}^d$ and involves an energy functional that contains gradient norms. Moreover, the minimizing sequence may not be compact due to escape at infinity. Such problems are often called locally compact variational problems [29]. Indeed, the main difficulty comes from the constraint, i.e., a sequence γ_n may satisfy the conditions in (1.6) and converge to some γ_∞ that in general has the correct energy $E_{\text{hf}}(N)$ but $\text{Tr}_{\mathfrak{H}}\{\gamma_\infty\}$ is strictly inferior to N. It is worth mentioning here that in most cases the energy functional is weakly lower semi-continuous in the $H^1(\mathbb{R}^d)$ topology. Further, as explained in [18], spectral theory plays an important role at some points by studying the simple quadratic case

$$E = \inf\Big\{\langle\Phi|(-\triangle + V)\Phi\rangle\,\Big|\,\Phi \in H^1(\mathbb{R}^3),\ \int\limits_{\mathbb{R}^3} |\Phi(x)|^2\,dx = 1\Big\}. \tag{1.9}$$

In the non-linear case at hand, the Schrödinger operator $-\triangle + V$ depends on the molecular orbitals φ_i which correspond to an N-body wave function Φ in the anti-symmetric product $\mathcal{H}$. Therefore, it is essential to know whether the potential V is positive or negative. Furthermore, uniqueness of the minimizer is not known even in cases where it is expected, and the minimizer does not need to be unique. For example we can take $N = 1$, then the difference between the direct term and exchange term is zero, i.e.,

$$\text{Tr}_{\mathfrak{H}\otimes\mathfrak{H}}\Big\{W(1 - \text{Ex})(\gamma \otimes \gamma)\Big\} = 0. \tag{1.10}$$

Therefore, the minimizer in this case is simply the projection onto a ground state of the operator h on the space $\mathfrak{H}$. Since the spin can point in any direction many ground states are available. The HF minimization problem has been studied by Lieb and Simon 1974 in [19], where they proved the following theorems about the existence of minimizers.

Theorem 1.2 (Existence of HF minimizers)**.** *If N is a positive integer such that $N < Z+1$ then there exists an N-dimensional projection γ minimizing the functional $\mathcal{E}_{\text{hf}}$ in (1.5), i.e., $E_{\text{hf}}(N) = \mathcal{E}_{\text{hf}}(\gamma)$ is a minimum.*

Note that Theorem 1.2 is about unrestricted HF-theory, i.e., the spatial functions for spin up and spin down are different. The single particle functions of space and spin φ_i are complex valued and not restricted to products of functions of space and functions of spin. They do not need to have any definite rotational symmetry in the atomic case. In the opposite case Lieb [17] has shown that there is no embedded eigenvalue for atoms with N electrons and nuclear charge Z, provided $N \geq 2Z + 1$, more precisely:

Theorem 1.3. *If N is a positive integer such that $N \geq 2Z + 1$, there are no minimizers for the HF functional among N-dimensional projections, i.e., there does not exist a rank N projection γ such that $E_{\mathrm{hf}}(N) = \mathcal{E}_{\mathrm{hf}}(\gamma)$.*

This result is very good for $Z = 1$, but it is far from optimal for large Z. It was improved by Solovej in [28], who proved the ionization conjecture.

Theorem 1.4. *There exists a universal constant $Q > 0$ such that for all positive integers satisfying $N > Z + Q$ there are no minimizers for the HF functional among the N-dimensional projections.*

In [7] Enstedt and Melgaard have shown that, if one imposes that

1. the vector potential A lies in $L^4_{\mathrm{loc}}(\mathbb{R}^3, \mathbb{R}^3)$ and its divergence ∇A lies in $L^2_{\mathrm{loc}}(\mathbb{R}^3)$, and
2. there exists some $R > 0$ such that the vector potential A is dominated by a positively homogeneous function of degree $s \in (-\infty, 0)$ for $|x| > R$,

then there are no minimizers for the magnetic HF problem when $N \geq 2Z + K$, where K is the number of the nuclei. If the minimizer satisfies the HF equations, then these equations state that a minimizing N-dimensional projection γ is the projection onto the N-dimensional space spanned by eigenfunctions φ_i with lowest possible eigenvalues ε_i for the HF mean field operator H_{hf} which is defined by

$$H_{\mathrm{hf}} := -\triangle - Z \cdot |x|^{-1} + \rho_\gamma * |x|^{-1} - \mathrm{Ex}_\gamma,$$

where the exchange operator Ex_γ is defined by the integral kernel

$$\mathrm{Ex}_\gamma(x, y) = |x - y|^{-1} \gamma(x, y),$$

where $\gamma(x, y)$ is defined later in (1.12) and

$$H_{\mathrm{hf}} \varphi_i = \varepsilon_i \varphi_i,$$

with $\varepsilon_1, \dots, \varepsilon_n \leq 0$ being the N lowest eigenvalues of H_{hf} (counting their multiplicity) corresponding to the eigenfunctions φ_i. This fact was stated in the following theorem and proven in [28].

Theorem 1.5. *If γ with density ρ_γ is a projection minimizing the HF functional $\mathcal{E}_{\mathrm{hf}}$ under the constraint $\mathrm{Tr}\,(\gamma) = N$, then $\rho_\gamma \in L^{\frac{5}{3}}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$ and H_{hf} defines a semibounded self-adjoint operator with the form domain $H^1(\mathbb{R}^3; \mathbb{C}^2)$ having at least N non-positive eigenvalues. Moreover, γ minimizes $\gamma \longmapsto \mathrm{Tr}_{\mathfrak{H}}\{H_{\mathrm{hf}}\gamma\}$ among all 1-pdm with $\mathrm{Tr}\,(\gamma) = N$.*

The functions $\varphi_1, \ldots, \varphi_N$ comprising the energy-minimizing Slater determinant Φ occupy the N lowest energy levels of H_{hf}, as was noted in [34] as a consequence of the following theorem:

Theorem 1.6. *Assume that W is positive definite, i.e., for every nonzero function φ of two space-spin variables we have*

$$\sum_{\sigma,\sigma'=\pm 1} \int |\varphi(r,\sigma;r',\sigma')|^2 \, W(r,\sigma;r',\sigma')\, d^3r\, d^3r' > 0.$$

Let φ be an eigenfunction of the operator H_{hf} defined by

$$\begin{aligned}(H_{\mathrm{hf}} f)(r,\sigma) = {} & (-\triangle - Z\,|x|^{-1} + \int \sum_{\tau=\pm 1} \sum_{j=1}^{N} |\varphi_j(r',\tau)|^2 \, W(r,\sigma;r',\tau) d^3r') f(r,\sigma) \\ & - \sum_{\tau=\pm 1} \sum_{j=1}^{N} \varphi_j(r,\sigma) \int \overline{\varphi_j(r',\tau)}\, f(r',\tau)\, W(r,\sigma;r',\tau)\, d^3r',\end{aligned}$$

with eigenvalue ε (i.e., $H_{\mathrm{hf}}\varphi = \varepsilon\varphi$) that is orthogonal to the minimizing set $\varphi_1, \ldots, \varphi_N$, i.e., $\langle \varphi | \varphi_k \rangle = 0$ for all $1 \le k \le N$. Then $\varepsilon > \varepsilon_k$ for all $1 \le k \le N$.

Another consequence of this theorem, which will be used many times is the following: the Slater determinant Φ, defined through the functions φ_i, minimizes the energy functional and does not leave any degenerate level unfilled. Since $\varepsilon > \varepsilon_k$ for all $k = 1, 2, \ldots, N$, we deduce that there is a gap between the eigenvalue ε and the k^{th} eigenvalue of the HF Hamiltonian. The idea of the proof is based on contradiction: it is assumed that the level is not filled and the remaining eigenfunctions of the HF operator are used to construct a new Slater determinant which has a strictly lower energy than the HF ground state.

1.2 Periodic Hartree-Fock Theory

Before the periodic problem is introduced we refer to the Appendix C, in which some definitions related to lattices in the Euclidean space $\mathbb{R}^d$ are recalled, which play a major role in this context. In the periodic case, the Hilbert space

$$\mathfrak{H}_\Lambda := L^2(\Lambda) \otimes \mathbb{C}^2 = L^2\Big\{\mathbb{R}^d/(L\mathbb{Z})^d\Big\} \otimes \mathbb{C}^2,$$

where the length L is an integer and a periodic density matrix γ_{per} are considered. γ_{per} is a self-adjoint operator on the physical space $\mathfrak{H}_\Lambda$ with eigenvalues between zero and one. It still describes a state of the system and models a finite number of electrons if $\mathrm{Tr}\,(\gamma_{\mathrm{per}}) < \infty$. Further it commutes with translation operators on $\mathfrak{H}_\Lambda$ by vectors of the lattice $\Gamma := \mathbb{Z}^d$. Also the potential V is assumed to be a Γ-periodic function, i.e., $V(x+k) = V(x)$ for all $k \in \Gamma$ and $x \in \Lambda$. This periodicity of γ_{per} and V means that the density of electrons, which move under the effect of the same potential V, in each unit cell $Q = \Lambda/\Gamma$ is equal. In the periodic setting, there is also a HF energy functional depending on γ_{per} , see formula (1.15) below. It was proved by Catto, Le Bris and Lions [14] that this energy admits a minimizer and by Lewin and Ghimenti [10] that any minimizer γ of the periodic HF energy is a projector and solves an equation of the form

$$\gamma_{\mathrm{per}} = \mathbb{1}\left[H_{\mathrm{hf}}(\gamma_{\mathrm{per}}) < \mu\right] + \varepsilon \;\; \mathbb{1}\left[H_{\mathrm{hf}}(\gamma_{\mathrm{per}}) = \mu\right]$$

with $\varepsilon \in \{0,1\}$ and $\mu \in \mathbb{R}$. The spectrum of H_{hf} is composed of bands and μ may be an eigenvalue (of infinite multiplicity, due to the invariance by translations of the lattice).

1.2.1 The Periodic Hartree-Fock Functional

The HF functional depends on the periodic one-particle (per-1-pdm) density matrix of the electrons, the main object of interest in the periodic problem. The 1-pdm represent the states of the electrons, over which the HF functional will be optimized. Since the periodic HF ground state energy is of great interest, to define it we introduce the set of per-1-pdm. Let τ_k for $k \in \Gamma$ be the translation operator on $\mathfrak{H}_\Lambda$ defined by

$$(\tau_k\,\varphi)\,(x) = \varphi(x+k).$$

If $(\tau_k\,\varphi)\,(x) = \varphi(x)$ we say that the function $\varphi \in \mathfrak{H}_\Lambda$ is Γ-periodic. Moreover, if any operator K on $\mathfrak{H}_\Lambda$ satisfies that $\tau_k\,K = K\,\tau_k$ for every $k \in \Gamma$, we say also that the operator K is Γ-periodic. Then the set

$$P_{\mathrm{per}}^{(N)} := \left\{\gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda)\,\middle|\, 0 \le \gamma \le \mathbb{1},\, \mathrm{Tr}\,(\gamma) = N, \mathrm{Tr}\,\{h\gamma\} < \infty,\, \tau_k\gamma = \gamma\tau_k,\, \forall k \in \Gamma\right\}, \tag{1.11}$$

is called the set of per-1-pdm, on which the HF functional $\mathcal{E}_{\mathrm{hf}}$ is defined. Here, h is the one-particle operator of the physical system under consideration acting on $\mathfrak{H}_\Lambda$. The kernel of $\gamma \in P_{\mathrm{per}}^{(N)}$ may be written as

$$\gamma(x,\sigma;y,\tau) = \sum_{\sigma,\tau=\pm}\sum_{j\ge 1}\lambda_j\,\overline{\varphi_j(x,\sigma)}\,\varphi_j(y,\tau), \tag{1.12}$$

and its density ρ_γ is the non-negative Γ-periodic function of $L^1(\Lambda;\mathbb{C}^2)$ defined by $\rho_\gamma(x,\sigma)=\gamma(x,\sigma;x,\sigma)$. Notice that, for any $\gamma\in P_{\mathrm{per}}^{(N)}$, we have

$$\sum_{\sigma=\pm}\int_\Lambda \rho_\gamma(x,\sigma)dx=\mathrm{Tr}\,(\gamma)=N, \tag{1.13}$$

i.e., (1.13) gives the total number of electrons in Λ. The non-relativistic quantum mechanical model for an atom or molecule is given by the Hamiltonian

$$H_N^{(g)}:=\sum_{i=1}^N h_i+g\sum_{1\le i<j\le N}W_{i,j} \tag{1.14}$$

acting as a self-adjoint operator on a dense domain $D_N\subseteq\bigwedge_{i=1}^N\mathfrak{H}_\Lambda$.
Here for every $i\in\{1,\ldots,N\}$, h_i is again the one-particle operator acting on $\mathfrak{H}_\Lambda$, $W_{i,j}:=W(x_i-x_j)\ge 0$ for every $i,j\in\{1,\ldots,N\}$ is a repulsive pair interaction potential acting on $\mathfrak{H}_\Lambda\otimes\mathfrak{H}_\Lambda$ and g is a small coupling constant ($0<g\ll 1$), i.e., a positive number that determines the strength of the interaction. The HF functional is then defined by

$$\mathcal{E}_{\mathrm{hf}}(\gamma):=T(\gamma)+\frac{g}{2}Q(\gamma,\gamma), \tag{1.15}$$

with

$$T(\gamma)=\mathrm{Tr}_{\mathfrak{H}_\Lambda}\{h\,\gamma\},$$

linear in $\gamma\in P_{\mathrm{per}}^{(N)}$ and the quadratic form

$$Q(\gamma,\eta)=\sum_{\sigma,\tau=\pm}\int\!\!\int_{\Lambda\times\Lambda}\left\{\overline{\gamma(x,\sigma;x,\sigma)}\,\eta(y,\tau;y,\tau)-\overline{\gamma(x,\sigma;y,\tau)}\,\eta(x,\sigma;y,\tau)\right\}W(x,\sigma;y,\tau)\,dx\,dy, \tag{1.16}$$

which is sesquilinear in $(\gamma,\eta)\in P_{\mathrm{per}}^{(N)}\times P_{\mathrm{per}}^{(N)}$. This functional defines the periodic HF energy as

$$E_{\mathrm{hf}}^{\mathrm{per}}(N):=\inf\left\{\mathcal{E}_{\mathrm{hf}}(\gamma)\,\middle|\,\gamma\in P_{\mathrm{per}}^{(N)}\right\}, \tag{1.17}$$

which is obviously greater than, or equal to, the non-periodic HF energy

$$E_{\mathrm{hf}}(N)=\inf\left\{\mathcal{E}_{\mathrm{hf}}(\gamma)\,\middle|\,\gamma=\gamma^*=\gamma^2,\mathrm{Tr}(\gamma)=N,\mathrm{Tr}\{h\,\gamma\}<\infty\right\}.$$

Remark 1.1. If a variable number of particles is of interest, the chemical potential μ can be introduced so that the periodic HF minimization problem reads as follows

$$E_{\mathrm{hf},\mu}^{\mathrm{per}}(N):=\inf\left\{\mathcal{E}_{\mathrm{hf},\mu}(\gamma)\,\middle|\,\gamma\in P_{\mathrm{per}}\right\},$$

where the HF functional with chemical potential μ is given by

$$\mathcal{E}_{\mathrm{hf},\mu}(\gamma) := \mathcal{E}_{\mathrm{hf}}(\gamma) - \mu \operatorname{Tr}(\gamma) .$$

and the variation set of per-1-pdm is defined by

$$P_{\mathrm{per}} := \Big\{ \gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda) \Big| \, 0 \leq \gamma \leq \mathbb{1}, \operatorname{Tr}(\gamma) < \infty, \operatorname{Tr}_{\mathfrak{H}_\Lambda}\{h\,\gamma\} < \infty, \tau_k\gamma = \gamma\tau_k, \forall k \in \Gamma \Big\}.$$

Chapter 2

Periodic Minimizers of the Hartree-Fock Functional and Their Properties

Contents

Summary

Now we study the periodic case, modeling an infinite quantum crystal. For the sake of simplicity it will be assumed that the crystal is simply the lattice $\Gamma = \mathbb{Z}^d$ and that there is only one nucleus of charge Z at each site of Γ. Also the spin of the electrons will be ignored, as this does not modify the general case. In this work the periodic minimization problem defined by (1.14), (1.15) and (1.17) will be proved as well-defined, following the work of Catto, Le Bris and Lions in [14]; some of the arguments are also similar to those used by Lieb, Solovej and Yngvason in [5]. Moreover, any minimizer of the HF energy over periodic matrices for an N-particle system is shown to be equal to the projection onto the N lowest eigenvalues of the effective Hamiltonian. Our proof follows that given by Bach, Fröhlich and Jonsson in [33] adapted to the periodic case. Further, we prove that there is a gap in the

spectrum of the effective Hamiltonian above the energy level number N. This gap can be estimated by the interaction potential parametrized by a coupling constant g following the work [34]. This estimate plays an important role when we consider the periodic minimizer in the minimization problem for general matrices. We then use the contraction mapping principle, the assumption on the spectral gap of h to have a positive size and the self-consistent equation on the periodic minimizer arising from the fact that this minimizer is a projection related to the effective Hamiltonian to prove the uniqueness of the minimizer of the HF functional $\mathcal{E}_{\mathrm{hf}}$ on periodic matrices. This idea of the proof is also used in the paper of Griesemer and Hantsch [11] on unique solutions to the HF equations for closed shell atoms. In the next step we use a perturbation argument to show that this minimizer is in fact a minimizer of $\mathcal{E}_{\mathrm{hf}}$ for all density matrices without the periodicity constraint. Here the linearization of the energy around the periodic minimizer involves the effective Hamiltonian and therefore the presence of the gap in the spectrum of the effective Hamiltonian implies that the energy is increased by moving away from the periodic minimizer, even in the set of non-periodic matrices.

2.1 Properties of Periodic HF Minimizers

Our main result is the following:

Theorem 2.1. *Let $H_N^{(g)}$, $\mathcal{E}_{\mathrm{hf}}(\gamma)$ and $E_{\mathrm{hf}}^{\mathrm{per}}$ be as in* (1.14), (1.15) *and* (1.17), *$h := -\Delta + V$ and $\gamma_{\mathrm{per}} \in P_{\mathrm{per}}^{(N)}$. Moreover, we assume that the external potential $V \in L^2(\Lambda)$ is a symmetric and a relatively compact perturbation of $-\Delta$ and that the repulsive pair-interaction potential W satisfies*

$$\forall z \in \Lambda : |W(z)| \leq \frac{c}{d_\Lambda(z)} \,,$$

where $d_\Lambda : \Lambda \longrightarrow \mathbb{R}_0^+$ with $d_\Lambda(z) := \inf\Big\{|z + Lq| \,\Big|\, q \in \mathbb{Z}^d\Big\}$ defines a metric on Λ and $c < \infty$ is a suitable constant. Then

1. *the HF functional $\mathcal{E}_{\mathrm{hf}}(\gamma)$ is well-defined and bounded from below on $P_{\mathrm{per}}^{(N)}$. Moreover, there exists a minimizer γ_{per} of the minimization problem defined in* (1.17).

2. *γ_{per} fulfills the self-consistent equation*

$$\gamma_{\mathrm{per}} = \mathbb{1}\left[H_{\mathrm{eff}}^{(g)}\left(\gamma_{\mathrm{per}}\right) \leq e_N\right],$$

where e_N is the N^{th} eigenvalue of the effective Hamiltonian defined by

$$\left[H_{\text{eff}}^{(g)}\left(\gamma_{\text{per}}\right)\psi\right](x) = [h\psi](x) + g\int_{\Lambda}\left\{\gamma_{\text{per}}(y,y)\psi(x) - \overline{\gamma_{\text{per}}(x,y)}\psi(y)\right\}W(x-y)dy, \quad (2.1)$$

for all $\psi \in \mathfrak{H}_\Lambda$.

3. *there is a gap in the spectrum of the effective Hamiltonian defined in* (2.1) *above the energy level number N.*

4. *assume that the N^{th} eigenvalue of h is separated by a gap of size $2a$, with $a > 0$, from the rest of the spectrum, then γ_{per} is unique on $P_{\text{per}}^{(N)}$.*

5. *under the same assumption as in 4, γ_{per} is a minimizer of $\mathcal{E}_{\text{hf}}$ over all density matrices without the periodicity constraint. In particular $E_{\text{hf}}^{\text{per}}(N) = E_{\text{hf}}(N)$.*

2.1.1 Existence of Periodic Minimizers of the HF Functional

We start with the proof of the existence of the minimizer in the variation set $P_{\text{per}}^{(N)}$.

Theorem 2.2. *Let $d \geq 3$ and $h := -\Delta + V$, where $-\Delta$ is the Laplace operator on $\mathfrak{H}_\Lambda$ and $V \in L^2(\Lambda)$ defines the external potential, which is a symmetric and a relatively compact perturbation of $-\Delta$. Suppose, moreover, that for all $z \in \Lambda$*

$$|W(z)| \leq \frac{c}{d_\Lambda(z)}\,, \quad (2.2)$$

where $d_\Lambda : \Lambda \longrightarrow \mathbb{R}_0^+$ with $d_\Lambda(z) := \inf\left\{|z+Lq| \,\middle|\, q \in \mathbb{Z}^d\right\}$ defines a metric on Λ and $c < \infty$ is a suitable constant. Then the Γ-periodic minimization problem defined by (1.14)*,* (1.15) *and* (1.17) *attains its minimum.*

The proof of Theorem 2.2 is too long, therefore we divide it into the following lemmas.

Lemma 2.1. *The set of per-1-pdm $P_{\text{per}}^{(N)}$ given in* (1.11) *is closed in the weak* topology* [1]*.*

Proof. To set up the variational problem, we define a class of HF states having finite trace and finite kinetic energy. Therefore we introduce the following complex Banach space of density matrices

$$X := \left\{\gamma \in \mathscr{L}^1\left(\mathfrak{H}_\Lambda\right) \mid 0 \leq \gamma \leq \mathbb{1}, \|\gamma\|_X < \infty\right\},$$

[1] Let X^* be the dual of the Banach space X. The weak* topology is the weakest topology on X^* in which all the functions $\ell \longmapsto \ell(x)$, $x \in X$, are continuous.

equipped with the norm

$$\begin{aligned}\|\gamma\|_X &:= \left\|(1-\Delta)^{\frac{1}{2}}\,\gamma^{\frac{1}{2}}\right\|_{HS}^2 \\ &= \operatorname{Tr}\left\{(1-\Delta)^{1/2}\gamma(1-\Delta)^{1/2}\right\}.\end{aligned}$$

Furthermore we remark that $P_{\text{per}}^{(N)}$ is a subset of X,

$$P_{\text{per}}^{(N)} = \left\{\gamma \in X \,\middle|\, \operatorname{Tr}_{L^2(\Lambda)}(\gamma) = N,\ \forall k \in \Gamma : \tau_k\gamma = \gamma\tau_k\right\}. \tag{2.3}$$

Note that $P_{\text{per}}^{(N)}$ is a convex subset of X. We now provide a topology for X as follows: the fact that the space of trace class operators, $\mathscr{L}^1(\mathfrak{H}_\Lambda)$, is the dual space of the space of compact operators, $\mathscr{K}(\mathfrak{H}_\Lambda)$ [2], (see [27] or [36]) naturally induces a weak* topology on X, for which the closed unit ball is compact, by the Banach-Alaoglu theorem [25]. More precisely, we say that γ_n converges weakly* to γ in X, $W_X^*\text{-}\lim_{n\to\infty}\gamma_n = \gamma$, if

$$\operatorname{Tr}_{L^2(\Lambda)}\{(1-\Delta)^{1/2}\,\gamma_n\,(1-\Delta)^{1/2}K\} \longrightarrow \operatorname{Tr}_{L^2(\Lambda)}\{(1-\Delta)^{1/2}\,\gamma\,(1-\Delta)^{1/2}\,K\}, \tag{2.4}$$

as $n \longrightarrow \infty$, for all compact operators K. Furthermore we remark that the inequality

$$\operatorname{Tr}_{L^2(\Lambda)}(\gamma) < \liminf_{n\longrightarrow\infty} \operatorname{Tr}_{L^2(\Lambda)}(\gamma_n)$$

cannot occur in our case. We have

$$\left|\operatorname{Tr}\left\{\gamma_n - \gamma\right\}\right| \le \left|\operatorname{Tr}\left\{K_M\left(\gamma_n-\gamma\right)\right\}\right| + \left|\operatorname{Tr}\left\{K_M^\perp\,\gamma_n\right\}\right| + \left|\operatorname{Tr}\left\{K_M^\perp\,\gamma\right\}\right|,$$

wobei $K_M = \mathbb{1}\,[h \le M]$ for some $M > 0$ such that dim Ran $K_M < \infty$. Moreover,

$$\operatorname{Tr}\left\{K_M^\perp\,\gamma_n\right\} \le \operatorname{Tr}\left\{\mathbb{1}\left[h > M\right]\,\frac{h}{M}\,\gamma_n\right\} \le \frac{1}{M}\,\operatorname{Tr}\left\{h\,\gamma_n\right\} \le \frac{R}{M},$$

since $\operatorname{Tr}\left\{h\,\gamma_n\right\} \le R < \infty$. Similarly, $\operatorname{Tr}\left\{K_M^\perp\,\gamma\right\} \le \frac{R}{M}$. Therefore,

$$\left|\operatorname{Tr}\left\{\gamma_n - \gamma\right\}\right| \le \left|\operatorname{Tr}\left\{K_M\left(\gamma_n-\gamma\right)\right\}\right| + 2\frac{R}{M}.$$

If M is big enough, then $2\frac{R}{M} < \frac{\varepsilon}{2}$. Suppose now M is fixed and n is big enough, then according to (2.4) we have $\left|\operatorname{Tr}\left\{K_M\left(\gamma_n-\gamma\right)\right\}\right| < \frac{\varepsilon}{2}$. This yields

$$\left|\operatorname{Tr}\left\{\gamma_n - \gamma\right\}\right| < \varepsilon.$$

[2] For a separable Hilbert space $\mathfrak{H}$, the nuclear operators $N_1(\mathfrak{H})$ are the trace-class operators $\mathscr{L}^1(\mathfrak{H})$, including the norm. Moreover $N_1(\mathfrak{H})$ is the dual space of the compact operators $\mathscr{K}(\mathfrak{H}_\Lambda)$.

Therefore the weak* limit for any net $\left\{\gamma_n\right\}_{n\in I} \subseteq P_{\mathrm{per}}^{(N)}$ for a directed system I, is again in $P_{\mathrm{per}}^{(N)}$, i.e.,

$$P_{\mathrm{per}}^{(N)} \text{ is closed in the weak* topology on } X.$$

$\square$

In order to check that the minimization problem (1.14), (1.15) and (1.17) admits a minimum, we can use the weak* compactness Theorem [29]. We must also check the following.

1. $\mathcal{E}_{\mathrm{hf}}$ is (sequentially) weakly* lower semi-continuous on $P_{\mathrm{per}}^{(N)}$ with respect to X, i.e., for any $\gamma \in P_{\mathrm{per}}^{(N)}$ and any net γ_n in $P_{\mathrm{per}}^{(N)}$ which converges weakly* to γ in X, it holds true that
$$\mathcal{E}_{\mathrm{hf}}(\gamma) \leq \liminf_{n\longrightarrow\infty} \mathcal{E}_{\mathrm{hf}}\left(\gamma_n\right).$$
2. $\mathcal{E}_{\mathrm{hf}} : P_{\mathrm{per}}^{(N)} \longrightarrow \mathbb{R}\cup\{\infty\}$ is coercive, i.e., $\mathcal{E}_{\mathrm{hf}}(\gamma_n) \longrightarrow \infty$, as $\|\gamma_n\|_X \longrightarrow \infty$, for $n \longrightarrow \infty$, $\gamma_n \in P_{\mathrm{per}}^{(N)}$.

Lemma 2.2. *Let $d \geq 3$, $P_{\mathrm{per}}^{(N)}$ be as in (2.3) and $V \in L^2(\Lambda)$ be a symmetric and a relatively compact perturbation of the Laplace operator $-\Delta$ on $\mathfrak{H}_\Lambda$. Suppose, moreover, for all $z \in \Lambda$*

$$|W(z)| \leq \frac{c}{d_\Lambda(z)}, \tag{2.5}$$

where $d_\Lambda : \Lambda \longrightarrow \mathbb{R}_0^+$, with $d_\Lambda(z) := \inf\left\{|z+Lq| \,\middle|\, q\in\mathbb{Z}^d\right\}$, defines a metric on Λ and $c<\infty$ is a suitable constant. Then the HF functional

$$\mathcal{E}_{\mathrm{hf}} : P_{\mathrm{per}}^{(N)} \longrightarrow \mathbb{R}\cup\left\{+\infty\right\}$$

is (sequentially) weakly lower semi-continuous on $P_{\mathrm{per}}^{(N)}$, i.e.,*

$$\mathcal{E}_{\mathrm{hf}}(\gamma) \leq \liminf_{n\longrightarrow\infty} \mathcal{E}_{\mathrm{hf}}\left(\gamma_n\right).$$

Let us remark that we have on purpose chosen a strategy of proof that extends to the entire space $\mathbb{R}^d$.

Proof. In the following we show, using Arazy's theorem [[27],Thm A.6], that for any net of operators $\left(\gamma_n\right)_{n\in I} \subseteq P_{\mathrm{per}}^{(N)}$ such that

$$\mathcal{E}_{\mathrm{hf}}(\gamma_n) \to E_{\mathrm{hf}}^{\mathrm{per}}(N),$$

as $n \longrightarrow \infty$, we have that $(\gamma_n)_{n \in I}$, after passing to a subnet if necessary, converges strongly to some operator $\gamma \in P_{\mathrm{per}}^{(N)}$ with $\mathcal{E}_{\mathrm{hf}}(\gamma) = E_{\mathrm{hf}}^{\mathrm{per}}(N)$. First we remark that, for every $n \in I$, there is an orthonormal basis $\left\{\varphi_j^{(n)}\right\}_{j \in \mathbb{N}} \subseteq \mathfrak{H}_\Lambda$ and $\left\{\lambda_j^{(n)}\right\}_{j \in \mathbb{N}} \subseteq [0,1]$ with $\sum\limits_{j=1}^{\infty} \lambda_j^{(n)} = N$ such that

$$\gamma_n = \sum_{j=1}^{\infty} \lambda_j^{(n)} |\varphi_j^{(n)}\rangle\langle\varphi_j^{(n)}|.$$

We denote by

$$\gamma_n(x,y) = \sum_{j=1}^{\infty} \lambda_j^{(n)} \overline{\varphi_j^{(n)}(x)} \varphi_j^{(n)}(y),$$

the Schwarz kernel of γ_n. Next, we note

$$\begin{aligned}
\int_\Lambda \int_\Lambda |\gamma_n(x,y)|^2 \, dx\, dy &= \int_\Lambda \int_\Lambda |\sum_{j=1}^{\infty} \lambda_j^{(n)} \, \overline{\varphi_j^{(n)}(x)} \, \varphi_j^{(n)}(y)|^2 dx\, dy \\
&= \int_\Lambda \int_\Lambda [\sum_{j=1}^{\infty} \lambda_j^{(n)} \, \overline{\varphi_j^{(n)}(x)} \, \varphi_j^{(n)}(y)] [\sum_{p=1}^{\infty} \lambda_p^{(n)} \varphi_p^{(n)}(x) \, \overline{\varphi_p^{(n)}(y)}] dx\, dy \\
&= \sum_{j,p=1}^{\infty} \lambda_j^{(n)} \lambda_p^{(n)} |\int_\Lambda \overline{\varphi_j^{(n)}(x)} \, \varphi_p^{(n)}(x) \, dx|^2,
\end{aligned}$$

where Lebesgue's dominated convergence theorem was used to obtain the last equation. Since $\left\{\varphi_j^{(n)}\right\}_{j \in \mathbb{N}} \subseteq \mathfrak{H}_\Lambda$ is an orthonormal basis we get

$$\int_\Lambda \int_\Lambda |\gamma_n(x,y)|^2 \, dx\, dy \leq \sum_{j=1}^{\infty} \left(\lambda_j^{(n)}\right)^2 \leq \sum_{j=1}^{\infty} \lambda_j^{(n)} = N < \infty,$$

whence

$$\gamma_n(x,y) \text{ is bounded in } L^2(\Lambda \times \Lambda).$$

Furthermore we have for each $n \in \mathbb{N}$,

$$\left\| \sqrt{\gamma_n(x,x)} \right\|_{H^1(\Lambda)}^2 = \int_\Lambda \left\{ \left| \nabla \sqrt{\gamma_n(x,x)} \right|^2 + \left| \sqrt{\gamma_n(x,x)} \right|^2 \right\} dx. \tag{2.6}$$

Here

$$\int_\Lambda \left|\gamma_n(x,x)\right| dx = \int_\Lambda \left| \sum_{j=1}^{\infty} \lambda_j^{(n)} \left|\varphi_j^{(n)}(x)\right|^2 \right| dx.$$

Since $\left\{\varphi_j^{(n)}\right\}_{j\in\mathbb{N}} \subseteq \mathfrak{H}_\Lambda$ is an orthonormal basis we get

$$\int\limits_{\Lambda} |\gamma_n(x,x)|\, dx = \sum_{j=1}^{\infty} \lambda_j^{(n)} = N < \infty. \tag{2.7}$$

Therefore,

$$\int\limits_{\Lambda} \left|\sqrt{\gamma_n(x,x)}\right|^2 dx < \infty.$$

For the second term on the right hand side of (2.6) we observe

$$\int\limits_{\Lambda} \left|\nabla\sqrt{\gamma_n(x,x)}\right|^2 dx = \int\limits_{\Lambda} \left|\nabla\Big(\sum_{j=1}^{\infty} \lambda_j^{(n)} \left|\varphi_j^{(n)}(x)\right|^2\Big)^{1/2}\right|^2 dx.$$

But for $\gamma_n(x,x) \neq 0$ we have

$$\begin{aligned}
\nabla_x\sqrt{\gamma_n(x,x)} &= \nabla_x\left\{\sqrt{\sum_{j=1}^{\infty} \lambda_j^{(n)} \overline{\varphi_j^{(n)}(x)}\varphi_j^{(n)}(x)}\right\} \\
&= \frac{1}{2\sqrt{\gamma_n(x,x)}} \sum_{j=1}^{\infty} \lambda_j^{(n)} \cdot 2\mathrm{Re}\left[\overline{\varphi_j^{(n)}(x)}\left(\nabla\varphi_j^{(n)}(x)\right)\right],
\end{aligned}$$

and therefore

$$\begin{aligned}
\left|\nabla_x\sqrt{\gamma_n(x,x)}\right|^2 &\leq \frac{1}{\gamma_n(x,x)} \Big(\sum_{j=1}^{\infty} \lambda_j^{(n)} |\varphi_j^{(n)}(x)|^2\Big)\Big(\sum_{j=1}^{\infty} \lambda_j^{(n)} \,|\nabla\varphi_j^{(n)}(x)|^2\Big) \\
&= \sum_{j=1}^{\infty} \lambda_j^{(n)} |\nabla\varphi_j^{(n)}(x)|^2,
\end{aligned}$$

which yields

$$\begin{aligned}
\int\limits_{\Lambda} \left|\nabla\sqrt{\gamma_n(x,x)}\right|^2 dx &\leq \int\limits_{\Lambda} \sum_{j\geq 1} \lambda_j^{(n)} \left|\nabla\,\varphi_j^{(n)}(x)\right|^2 dx. \\
&\leq \mathrm{Tr}_{L^2(\Lambda)}\{-\Delta\,\gamma_n\} \\
&\leq \mathrm{Tr}_{L^2(\Lambda)}\Big\{\Big(1-\Delta\Big)\gamma_n\Big\} < \infty,
\end{aligned} \tag{2.8}$$

since $(\gamma_n)_{n\in I} \subseteq P_{\mathrm{per}}^{(N)}$. Thus, the net

$$\left(\sqrt{\gamma_n(x,x)}\right)_{n\in I} \text{ is bounded in the Sobolev space } H^1(\Lambda). \tag{2.9}$$

By Rellich-Kondrachov theorem we deduce that $\sqrt{\gamma_n(x,x)}$ is bounded in $L^p(\Lambda)$, for all $1 \leq p < \frac{2d}{d-2}$ and all $n \in I$. This fact can also be expressed by stating that

$$\mathrm{Tr}_{L^2(\Lambda)}\left\{-\Delta\gamma_n\right\} = \int_\Lambda \sum_{j=1}^{\infty} \lambda_j^{(n)} \left|\nabla\varphi_j^{(n)}(x)\right|^2 dx, \tag{2.10}$$

is bounded uniformally in n. Using the Cauchy-Schwarz inequality as follows,

$$\begin{aligned}\left|\gamma_n(x,y)\right| &\leq \Big|\sum_{j=1}^{\infty} \lambda_j^{(n)} \overline{\varphi_j^{(n)}(x)}\varphi_j^{(n)}(y)\Big| \\ &\leq \Big(\sum_{j=1}^{\infty} \lambda_j^{(n)} \left|\varphi_j^{(n)}(x)\right|^2\Big)^{1/2}\Big(\sum_{j=1}^{\infty} \lambda_j^{(n)} \left|\varphi_j^{(n)}(y)\right|^2\Big)^{1/2} \\ &= \sqrt{\gamma_n(x,x)}\sqrt{\gamma_n(y,y)}, \end{aligned} \tag{2.11}$$

we obtain an explicit bound on $\gamma_n(x,y)$ for each n according to the bound (2.9), i.e.,

$$\gamma_n(x,y) \text{ is bounded in } H^1(\Lambda\times\Lambda), \text{ and thus in } L^p(\Lambda\times\Lambda),\ 1 \leq p < \frac{2d}{d-2}. \tag{2.12}$$

According to the bound (2.9) and the Banach-Alaoglu theorem in a Hilbert space [8],

$$\text{a subnet, which we a gain denote } \left\{\sqrt{\gamma_n(x,x)}\,\right\}_{n\in I},$$

$$\text{converges weakly in } H^1(\Lambda) \text{ to some function } \sqrt{\widetilde{\gamma}(x,x)}\ ^{3}.$$

Moreover, a uniformly bounded net in $H^1(\Lambda)$ has a subnet, again denoted $\left\{\sqrt{\gamma_n(x,x)}\right\}$ with $n \in I$, that converges strongly in $L^p(\Lambda), 1 \leq p < p^* = \frac{2d}{d-2}$ to a function $\sqrt{\widetilde{\gamma}(x,x)} \in L^p(\Lambda)$ due to the Rellich-Kondrachov Theorem [18], where there exists a constant $c \geq 0$ such that

$$\left\|\sqrt{\gamma_n(x,x)}\right\|_{L^p(\Lambda)} \leq c\left\|\sqrt{\gamma_n(x,x)}\right\|_{H^1(\Lambda)}.$$

As a consequence of the bounds come from (2.12). Again, we may assume that the net $\{\gamma_n(x,y)\}_{n\in I}$ converges weakly in $H^1(\Lambda\times\Lambda)$ and strongly in $L^p(\Lambda\times\Lambda)$, $1 \leq p < p^* = \frac{dp}{d-p}$, to some function $\gamma(x,y)$. From (2.9) and (2.11) we may also assume

[3] To prevent confusion, until now it does not represent a kernel of a compact operator.

that $\{(\nabla\gamma_n)(x,y)\}_{n\in I}$ with $(\nabla\gamma_n)(x,y) = \Big(\nabla_x\gamma_n, \nabla_y\gamma_n\Big)(x,y)$ converges weakly in $H^1(\Lambda\times\Lambda)$ to some function $\eta(x,y) \in H^1(\Lambda\times\Lambda)$. Moreover, by [[19],Thm 8.6] we emphasize that $\eta(x,y) = \nabla\gamma(x,y)$ for some unique function $\gamma(x,y) \in H^1(\Lambda\times\Lambda)$. Using Fatou's lemma gives

$$\liminf_{n\longrightarrow\infty} \mathrm{Tr}_{L^2(\Lambda)}\left\{-\Delta\gamma_n\right\} \geq \mathrm{Tr}_{L^2(\Lambda)}\left\{-\Delta\gamma\right\},$$

where this inequality is in fact an equality as a consequence of the dominated convergence theorem, since $\mathrm{Tr}\left\{-\Delta\gamma_n\right\}$ is bounded uniformly in n according to (2.10) and Theorem 8.7 in [18]. Testing the weak* convergence of γ_n with the compact operator $K = (1-\Delta)^{-1}$ (here we use that Λ is compact) yields

$$\begin{aligned}&\lim_{n\longrightarrow\infty} \mathrm{Tr}_{L^2(\Lambda)}\left\{(1-\Delta)^{1/2}\gamma_n(1-\Delta)^{1/2}(1-\Delta)^{-1}\right\}\\ &= \lim_{n\longrightarrow\infty} \mathrm{Tr}_{L^2(\Lambda)}\left\{(1-\Delta)^{1/2}\gamma(1-\Delta)^{1/2}(1-\Delta)^{-1}\right\},\end{aligned}$$

which may also be expressed as

$$\lim_{n\longrightarrow\infty} \mathrm{Tr}_{L^2(\Lambda)}\left(\gamma_n\right) = \mathrm{Tr}_{L^2(\Lambda)}\left(\gamma\right). \tag{2.13}$$

We can also write

$$\liminf_{n\longrightarrow\infty} \mathrm{Tr}_{L^2(\Lambda)}\left\{(1-\Delta)\gamma_n\right\} = \mathrm{Tr}_{L^2(\Lambda)}\left\{(1-\Delta)\gamma\right\}. \tag{2.14}$$

Thus, Arazy's theorem [[27],Thm A.6] implies that γ_n converges strongly to γ in $\mathscr{L}^1\left(\mathfrak{H}_\Lambda\right)$, provided that $\gamma(x,x) = \tilde{\gamma}(x,x)$. To this end, we choose the compact operator

$$A := (1-\Delta)^{-1/2}\, g(.)\, (1-\Delta)^{-1/2} \in \mathcal{K}(\mathfrak{H}_\Lambda),$$

defined for any bounded function $g(.)$ in $L^\infty(\Lambda)$. Using the definition of weak* convergence given in (2.4) we deduce on the one hand that

$$\begin{aligned}&\lim_{n\longrightarrow\infty} \mathrm{Tr}_{L^2(\Lambda)}\left[(1-\Delta)^{1/2}\gamma_n\,(1-\Delta)^{1/2}\,(1-\Delta)^{-1/2}\,g(.)\,(1-\Delta)^{-1/2}\right]\\ &= \mathrm{Tr}_{L^2(\Lambda)}\left[(1-\Delta)^{1/2}\gamma\,(1-\Delta)^{1/2}\,(1-\Delta)^{-1/2}\,g(.)\,(1-\Delta)^{-1/2}\right],\end{aligned}$$

which is equivalent to

$$\lim_{n\longrightarrow\infty} \int_\Lambda \gamma_n(x,x)\, g(x)\, dx = \int_\Lambda \gamma(x,x)\, g(x)\, dx.$$

On the other hand the Lieb-Thirring inequality in the periodic setting (see [30] for finite-rank projectors and [21] for its extension to general density matrices) yields

$$\int_{\Lambda} \gamma_n^{1+2/d}(x,x)dx \leq c_{LT}\mathrm{Tr}_{L^2(\Lambda)}\left\{(1-\Delta)\gamma_n\right\},$$

i.e., $\gamma_n(x,x)$ is bounded in $L^{1+2/d}(\Lambda)$, and as before we may assume that the net of non-negative functions $\{\gamma_n(x,x)\}_{n\in I}$ converges weakly in $L^{1+2/d}(\Lambda)$ to $\widetilde{\gamma}(x,x)$. Thus,

$$\lim_{n\longrightarrow\infty}\int_{\Lambda}\gamma_n(x,x)g(x)dx = \int_{\Lambda}\widetilde{\gamma}(x,x)g(x)dx.$$

We also get

$$\int_{\Lambda}\gamma(x,x)g(x)dx = \int_{\Lambda}\widetilde{\gamma}(x,x)g(x)dx.$$

Next, we show that the remaining terms in the HF functional are controlled by the kinetic energy. First, according to the Cauchy-Schwarz inequality we have

$$\left|\int_{\Lambda}V(x)\gamma_n(x,x)dx\right| \leq \|V\|_{L^2(\Lambda)}\|\gamma_n(x,x)\|_{L^2(\Lambda)}.$$

By the Hölder inequality and the boundedness of $\gamma_n(x,x)$ in $L^1(\Lambda)$, we obtain

$$\begin{aligned}\left|\int_{\Lambda}V(x)\gamma_n(x,x)dx\right| &\leq \|V\|_{L^2(\Lambda)}\|\gamma_n(x,x)\|_{L^1(\Lambda)}^{1/4}\|\gamma_n(x,x)\|_{L^3(\Lambda)}^{3/4} \\ &\leq N^{\frac{1}{4}}\|V\|_{L^2(\Lambda)}\|\gamma_n(x,x)\|_{L^3(\Lambda)}^{3/4}.\end{aligned}$$

Since Λ is a finite measure space, then $L^q\subset L^p$, for $1\leq p\leq q\leq\infty$. Moreover, using Rellich-Kondrachov, we get

$$\begin{aligned}\left|\int_{\Lambda}V(x)\gamma_n(x,x)dx\right| &\leq C\|V\|_{L^2(\Lambda)}\left\|\sqrt{\gamma_n(x,x)}\right\|_{H^1(\Lambda)}^{3/2} \\ &\leq C\|V\|_{L^2(\Lambda)}\left(N+\left\|\nabla\sqrt{\gamma_n(x,x)}\right\|_{L^2(\Lambda)}^2\right)^{3/4},\end{aligned}$$

which is controlled by the kinetic energy according to (2.9). Thanks to the strong convergence of γ_n in $\mathscr{L}^1(\mathfrak{H}_\Lambda)$ and to the Hardy-Littlewood-Sobolev inequality

$$\left|\int_{\Lambda}\int_{\Lambda}\gamma_n(x,x)|x-y|^{-1}\gamma_n(y,y)d^dxd^dy\right| \leq C(d,p)\|\gamma_n\|_p\|\gamma_n\|_r,$$

for $\frac{1}{p}+\frac{1}{r}=2-\frac{1}{d}$ and $p,r>1$ and since $|W(z)|\leq\frac{c}{d_\Lambda(z)}$ for some constant $c<\infty$ and for the metric $d_\Lambda:\Lambda\longrightarrow\mathbb{R}_0^+$ with $d_\Lambda(z):=\inf\left\{|z+Lq|\,\middle|\,q\in\mathbb{Z}^d\right\}$, we deduce that the direct term, $\int\limits_\Lambda\int\limits_\Lambda\gamma_n(x,x)\,W(x-y)\,\gamma_n(y,y)\,d^dx\,d^dy$, in the HF functional is bounded. Moreover by dominated convergence theorem we get,

$$\begin{aligned}&\lim_{n\longrightarrow\infty}\left[\int\limits_\Lambda V(x)\gamma_n(x,x)dx+\int\limits_\Lambda\int\limits_\Lambda\gamma_n(x,x)W(x-y)\gamma_n(y,y)dxdy\right]\\&=\int\limits_\Lambda V(x)\gamma(x,x)dx+\int\limits_\Lambda\int\limits_\Lambda\gamma(x,x)W(x-y)\gamma(y,y)dxdy.\end{aligned}$$

For the exchange term

$$\mathrm{Ex}(\gamma,\gamma)=\int\limits_\Lambda\int\limits_\Lambda W(x-y)\left|\gamma(x,y)\right|^2dxdy, \tag{2.15}$$

we have

$$\left|\int\limits_\Lambda\int\limits_\Lambda W(x-y)\left|\gamma_n(x,y)\right|^2dxdy\right|\leq\int\limits_\Lambda\int\limits_\Lambda\left|W(x-y)\right|\left|\gamma_n(x,y)\right|^2dxdy.$$

According to Assumption (2.5) we get

$$\left|\int\limits_\Lambda\int\limits_\Lambda W(x-y)\left|\gamma_n(x,y)\right|^2dxdy\right|\leq c\int\limits_\Lambda\int\limits_\Lambda\frac{1}{d_\Lambda(x-y)}\left|\gamma_n(x,y)\right|^2dxdy.$$

By the continuous Cauchy-Schwarz inequality we have proved in (2.11) that

$$\left|\gamma_n(x,y)\right|^2\leq\gamma_n(x,x)\gamma_n(y,y).$$

Therefore we can write

$$\left|\int\limits_\Lambda\int\limits_\Lambda W(x-y)\left|\gamma_n(x,y)\right|^2dxdy\right|\leq c\int\limits_\Lambda\int\limits_\Lambda\frac{\gamma_n(x,x)\gamma_n(y,y)}{d_\Lambda(x-y)}dxdy.$$

But we remark that

$$\int\limits_\Lambda\frac{\gamma_n(x,x)\gamma_n(y,y)}{d_\Lambda(x-y)}dy=\gamma_n(x,x)\left[\gamma_n(\cdot,\cdot)\star\frac{1}{d_\Lambda(\cdot)}\right](x),$$

where $\star$ denotes the convolution as a map from $\mathfrak{H}_\Lambda \times \mathfrak{H}_\Lambda$ to $\mathfrak{H}_\Lambda$. Thus, using Hölder's inequality for $p = 6$ and $q = \frac{6}{5}$ we obtain

$$\left| \int_\Lambda \int_\Lambda W(x-y) \left|\gamma_n(x,y)\right|^2 dx\, dy \right| \leq c \int_\Lambda \gamma_n(x,x) \left[\gamma_n(\cdot,\cdot) \star \frac{1}{d_\Lambda(\cdot)} \right](x) dx$$
$$\leq c \left\| \gamma_n(\cdot,\cdot) \star \frac{1}{d_\Lambda(x)} \right\|_{L^6(\Lambda)} \left\| \gamma_n(x,x) \right\|_{L^{6/5}(\Lambda)}.$$

Next, with Young's inequality for $p = 3$ and $q = \frac{6}{5}$ we get

$$\left| \int_\Lambda \int_\Lambda W(x-y) \left|\gamma_n(x,y)\right|^2 dx\, dy \right| \leq c \left\| \frac{1}{d_\Lambda(x)} \right\|_{L^3(\Lambda)} \left\| \gamma_n(x,x) \right\|^2_{L^{6/5}(\Lambda)}.$$

Again using Hölder's inequality for $p = 3$, $q = 2$ and $r = \frac{6}{5}$, then the Cauchy-Schwarz inequality on $\left\| \gamma_n(x,x) \right\|_2^2$ we deduce that

$$\left| \int_\Lambda \int_\Lambda W(x-y) \left|\gamma_n(x,y)\right|^2 dxdy \right| \leq c \left\| \frac{1}{d_\Lambda(x)} \right\|_{L^3(\Lambda)} \left\| \gamma_n(x,x) \right\|^2_{L^2(\Lambda)} \left\| \gamma_n(x,x) \right\|^2_{L^3(\Lambda)}$$
$$\leq cN^{1/2} \left\| \frac{1}{d_\Lambda(x)} \right\|_{L^3(\Lambda)} \left\| \gamma_n(x,x) \right\|^{3/2}_{L^3(\Lambda)} \left\| \gamma_n(x,x) \right\|^2_{L^3(\Lambda)}.$$

Since $\gamma_n(x,x) \in L^1(\Lambda)$ and $L^3(\Lambda) \subseteq L^1(\Lambda)$ in finite measure spaces we can write

$$\left| \int_\Lambda \int_\Lambda W(x-y) \left|\gamma_n(x,y)\right|^2 dxdy \right| \leq c_1 \left\| \frac{1}{d_\Lambda(x)} \right\|_{L^3(\Lambda)} \left\| \gamma_n(x,x) \right\|^{1/2}_{L^3(\Lambda)},$$

where $c_1 := cN^{1/2} \left\| \gamma_n(x,x) \right\|_3^3$. Finally we use the Rellich-Kondrachov theorem and (2.7) to deduce that

$$\left| \int_\Lambda \int_\Lambda W(x-y) \left|\gamma_n(x,y)\right|^2 dxdy \right| \leq c_2 \left\| \frac{1}{d_\Lambda(x)} \right\|_3 \left\| \sqrt{\gamma_n(x,x)} \right\|_{H^1(\Lambda)},$$

where $c_2 := 4c_1$. Using the definition of the metric d_Λ on Λ, the fact that $\gamma_n(x,x)$ is bounded in $L^1(\Lambda)$ and the definition of $\|.\|_{H^1(\Lambda)}$, then

$$\left| \int_\Lambda \int_\Lambda W(x-y) \left|\gamma_n(x,y)\right|^2 dxdy \right| \leq c_2 \left\| \frac{1}{d_\Lambda(x)} \right\|_3 \left(N + \left\| \nabla \sqrt{\gamma_n(x,x)} \right\|_{H^1(\Lambda)} \right)^{1/2}$$
$$\leq c_2 \left\| \frac{1}{|x|} \right\|_3 \left(N + \left\| \nabla \sqrt{\gamma_n(x,x)} \right\|_{H^1(\Lambda)} \right)^{1/2}, \tag{2.16}$$

which again implies that the exchange term is controlled by the kinetic energy. To get the limit of $\mathcal{E}_{\mathrm{hf}}(\gamma_n)$ we first apply the Cauchy-Schwarz inequality to obtain

$$\begin{aligned}
&\left| \int\limits_\Lambda \int\limits_\Lambda \left[|\gamma_n(x,y)|^2 - |\gamma(x,y)|^2 \right] \frac{c}{d_\Lambda(x-y)} dxdy \right| \\
&\leq C \left\| \frac{1}{d_\Lambda(x-y)} \right\|_{L^2(\Lambda)} \left\| |\gamma_n(x,y)|^2 - |\gamma(x,y)|^2 \right\|_{L^2(\Lambda)},
\end{aligned}$$

and then passing to the limit we obtain by dominated convergence

$$\lim_{n\longrightarrow\infty} \int\limits_\Lambda \int\limits_\Lambda W(x-y) \, |\gamma_n(x,y)|^2 \, dxdy = \int\limits_\Lambda \int\limits_\Lambda W(x-y) \, |\gamma(x,y)|^2 \, dxdy.$$

Thus, we have shown that

$$\lim_{n\longrightarrow\infty} \mathcal{E}_{\mathrm{hf}}(\gamma_n) = \mathcal{E}_{\mathrm{hf}}(\gamma) = E_{\mathrm{hf}}^{\mathrm{per}}(N),$$

with $\gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda)$. It remains to show that $\gamma \in P_{\mathrm{per}}^{(N)}$. Using (2.13) and the fact that $\mathrm{Tr}_{L^2(\Lambda)} \{\gamma_n\} = N$ we get $\mathrm{Tr}_{L^2(\Lambda)} (\gamma) = N$. Moreover,

$$\gamma_n \overset{\mathscr{L}^1(\mathfrak{H}_\Lambda)}{\longrightarrow} \gamma, \tag{2.17}$$

from which we conclude that $0 \leq \gamma \leq \mathbb{1}$, since $\gamma_n \in P_{\mathrm{per}}^{(N)}$ for each n. Furthermore, we have shown in (2.10) and (2.14) that

$$\begin{aligned}
&\mathrm{Tr}_{L^2(\Lambda)} \{(1-\Delta)\,\gamma_n\} \leq C \\
&\mathrm{Tr}_{L^2(\Lambda)} \{(1-\Delta)\ \gamma\} \leq \liminf_{n\longrightarrow\infty} \mathrm{Tr}_{L^2(\Lambda)} \{(1-\Delta)\,\gamma_n\},
\end{aligned}$$

which directly gives $\|\gamma\|_X < \infty$. Finally the invariance of γ with respect to the lattice Γ can be proven as follows: using (2.17) and the continuity of τ_k for each $k \in \Gamma$ we have

$$\tau_k\gamma_n \overset{\mathscr{L}^1(\mathfrak{H}_\Lambda)}{\longrightarrow} \tau_k\gamma \text{ and } \gamma_n\tau_k \overset{\mathscr{L}^1(\mathfrak{H}_\Lambda)}{\longrightarrow} \gamma\tau_k.$$

Since the limit in $\mathscr{L}^1(\mathfrak{H}_\Lambda)$ is unique and $\tau_k\gamma_n = \gamma_n\tau_k$ for each k and n, we get $\tau_k\gamma = \gamma\tau_k$ for every $k \in \Gamma$ and therefore $\gamma \in P_{\mathrm{per}}^{(N)}$. □

Remark 2.1. The proof given above from (2.15) to (2.16) to show that the exchange term is controlled by the kinetic energy can be achieved in one line, since the function

$W(z)$ is positive in our model and the exchange term is controlled by the direct term, i.e.,

$$\int_\Lambda\int_\Lambda W(x-y)\,|\gamma(x,y)|^2\,dx\;dy \leq \int_\Lambda\int_\Lambda W(x-y)\gamma(x,x)\gamma(y,y)\;dx\;dy,$$

However, this proof is satisfied in a general case, where the function $W(z)$ is not positive.

Lemma 2.3. *Let $P_{\mathrm{per}}^{(N)}$ be as in* (2.3) *and $V \in L^2(\Lambda)$ be a symmetric and a relatively compact perturbation of the Laplace operator $-\Delta$ on $\mathfrak{H}_\Lambda$. Suppose, moreover, for all $z \in \Lambda$ that*

$$|W(z)| \leq \frac{c}{d_\Lambda(z)}\,, \tag{2.18}$$

where $d_\Lambda : \Lambda \longrightarrow \mathbb{R}_0^+$ with $d_\Lambda(z) := \inf\Big\{|z+Lq|\,\Big|\, q \in \mathbb{Z}^d\Big\}$ defines a metric on Λ and $c < \infty$ is a suitable constant. Then the HF functional $\mathcal{E}_{\mathrm{hf}} : P_{\mathrm{per}}^{(N)} \longrightarrow \mathbb{R} \cup \{+\infty\}$ defined in (2.8) *is coercive.*

Proof. We note that the external potential V is $-\Delta$-bounded with relative bound smaller than 1 [4], the direct and the exchange terms in $\mathcal{E}_{\mathrm{hf}}$ are also controlled by the kinetic energy as shown in Lemma 2.2. Therefore, if

$$\|\gamma\|_X = \mathrm{Tr}\{(1-\Delta)\,\gamma\} \longrightarrow \infty, \text{ then clearly } \mathcal{E}_{\mathrm{hf}}(\gamma) \longrightarrow \infty.$$

□

2.1.2 Self-Consistent Equation

We now prove a result similar to [16] and [33]. Namely we show that any minimizer γ_{per} of the periodic HF functional on $P_{\mathrm{per}}^{(N)}$ is indeed a projection and it solves an equation of the form

$$\gamma_{\mathrm{per}} = \mathbb{1}\left[H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}}) \leq e_N\right],$$

where e_N is the N^{th} eigenvalue of the effective Hamiltonian. The fact that γ_{per} is a trace class operator is essential. We refer to [10] where the minimizer is no longer a trace class operator and commutes with translations by vectors of a given lattice. The authors have solved this problem by using the so-called Bloch wave decomposition, which gives a family of trace class operators for such a minimizer.

[4] relative compactness implies relative boundedness with relative bound zero.

Theorem 2.3. *Let $\gamma_{\text{per}} \in P_{\text{per}}^{(N)}$ be a minimizer of $\mathcal{E}_{\text{hf}}$. Then*

$$\gamma_{\text{per}} = \mathbb{1}\left[H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) \le e_N\right].$$

Before giving the proof of Theorem 2.3, the spectrum of the Hamiltonian $H_{\text{eff}}^{(g)}(\gamma)$ defined in (2.1) is analyzed in the following lemma

Lemma 2.4. *Let $d \le 3$, $N \in \mathbb{N}$, $0 < g \ll 1$, $P_{\text{per}}^{(N)}$ defined in* (2.3) *and $\gamma \in P_{\text{per}}^{(N)}$. We define $H_{\text{eff}}^{(g)}(\gamma)$ as in* (1.14) *and assume that the potential V is a symmetric and a relatively compact perturbation of $-\Delta$. Suppose, moreover for all $z \in \Lambda$ that*

$$|W(z)| \le \frac{c}{d_\Lambda(z)}\,, \tag{2.19}$$

where $d_\Lambda : \Lambda \longrightarrow \mathbb{R}_0^+$ with $d_\Lambda(z) := \inf\left\{|z + Lq| \,\middle|\, q \in \mathbb{Z}^d\right\}$ defines a metric on Λ and $c < \infty$ is a suitable constant. Then $H_{\text{eff}}^{(g)}(\gamma)$ is self-adjoint, bounded from below and has purely discrete spectrum.

Proof. $H_{\text{eff}}^{(g)}(\gamma)$ is self-adjoint, if the operator $\widetilde{V}$ defined by

$$\left(\widetilde{V}\varphi\right)(x) = g\int\limits_\Lambda \left\{\gamma(y,y)\varphi(x) - \overline{\gamma(x,y)}\varphi(y)\right\} W(x-y)dy \tag{2.20}$$

is a symmetric and a relatively compact perturbation of $-\Delta$ by Kato-Rellich theorem [15]. On the one hand

$$\begin{aligned}
\langle \widetilde{V}\varphi \mid \psi\rangle_{L^2(\Lambda)} &= \int\limits_\Lambda \overline{\left(\widetilde{V}\varphi\right)(x)}\psi(x)dx \\
&= g\int\limits_\Lambda \left[\int\limits_\Lambda \left\{\overline{\gamma(y,y)\varphi(x)} - \overline{\left(\overline{\gamma(x,y)}\right)\varphi(y)}\right\} \overline{W(x-y)}dy\right]\psi(x)dx \\
&= g\int\limits_\Lambda\int\limits_\Lambda \left\{\gamma(y,y)\overline{\varphi(x)} - \gamma(x,y)\overline{\varphi(y)}\right\} W(x-y)\psi(x)dx,
\end{aligned}$$

for all $\psi, \varphi \in \mathfrak{H}_\Lambda$, since $W(x)$ is real and γ is a self-adjoint operator. On the other hand

$$\begin{aligned}
\langle \varphi \mid \widetilde{V}\psi\rangle_{L^2(\Lambda)} &= \int\limits_\Lambda \overline{\varphi(x)}\left(\widetilde{V}\psi\right)(x)dx \\
&= g\int\limits_\Lambda \overline{\varphi(x)}\left[\int\limits_\Lambda \left\{\gamma(y,y)\psi(x) - \overline{\gamma(x,y)}\psi(y)\right\} W(x-y)dy\right]dx \\
&= g\int\limits_\Lambda\int\limits_\Lambda \left\{\gamma(y,y)\overline{\varphi(x)}\psi(x) - \overline{\gamma(y,x)\varphi(y)}\psi(x)\right\} W(y-x)dxdy.
\end{aligned}$$

The symmetry of $W(x)$ and the self-adjointness of γ imply

$$\left\langle \widetilde{V}\varphi \middle| \psi \right\rangle_{L^2(\Lambda)} = \left\langle \varphi \middle| \widetilde{V}\psi \right\rangle_{L^2(\Lambda)}.$$

Thus, the operator $\widetilde{V}$ is a symmetric. Moreover, the operator $\widetilde{V}$ is the sum of two operators:

1. the multiplication operator $\widetilde{V}_1$ defined by

$$\left(\widetilde{V}_1\varphi\right)(x) = V_1(x)\varphi(x),$$

where $V_1(x) := \int_\Lambda \gamma(y,y)W(x-y)dy = \left(\rho_\gamma \star W\right)(x)$, and

2. the integral operator $\widetilde{V}_2$ with kernel $V_2(x,y) = \overline{\gamma(x,y)}W(x-y)$.

To prove that $\widetilde{V}$ is a relatively compact perturbation of $-\Delta$ it must be shown that $\widetilde{V}_1(-\Delta+1)^{-1}$ and $\widetilde{V}_2(-\Delta+1)^{-1}$ are compact operators. For all $\phi \in \mathfrak{H}_\Lambda$ we have firstly

$$\begin{aligned}
\left[\widetilde{V}_1(-\Delta+1)^{-1}\phi\right](x) &= V_1(x)\left[(-\Delta+1)^{-1}\phi\right](x) \\
&= \int_\Lambda V_1(x)(-\Delta+1)^{-1}(y-x)\phi(y)dy \\
&= \int_\Lambda V_1(x)\,\mathcal{F}^{-1}\left[\frac{1}{p^2+1}\right](y-x)\phi(y)dy,
\end{aligned}$$

where $\mathcal{F} : \mathfrak{H}_\Lambda \longrightarrow \ell^2\left[(L\mathbb{Z})^d\right]$ is the Fourier transform. Thus, $\widetilde{V}_1(-\Delta+1)^{-1}$ is an integral operator with kernel

$$\left[\widetilde{V}_1(-\Delta+1)^{-1}\right](x,y) = V_1(x)\,\mathcal{F}^{-1}\left[\frac{1}{p^2+1}\right](y-x).$$

This yields

$$\begin{aligned}
&\int_\Lambda\int_\Lambda \left|\left[\widetilde{V}_1(-\Delta+1)^{-1}\right](x,y)\right|^2 dx\,dy \\
&= \int_\Lambda\int_\Lambda V_1(x)^2\left|\mathcal{F}^{-1}\left[\frac{1}{p^2+1}\right](y-x)\right|^2 dx\,dy \\
&= \left(\int_\Lambda V_1(x)^2 dx\right)\left(\int_\Lambda \left|\mathcal{F}^{-1}\left[\frac{1}{p^2+1}\right](y)\right|^2 dy\right).
\end{aligned}$$

Since $W \in L^2(\Lambda)$ and $\rho_\gamma \in L^1(\Lambda)$, hence $V_1 = \rho_\gamma * W \in L^2(\Lambda)$ and by Plancherel's theorem [26] we get

$$\int_\Lambda \int_\Lambda \left| \left[\widetilde{V}_1 (-\Delta + 1)^{-1} \right] (x,y) \right|^2 dx dy = \|V_1\|^2_{L^2(\Lambda)} \left\| \left(p^2 + 1 \right)^{-1} \right\|_{\ell^2\left[(L\mathbb{Z})^d\right]} < \infty,$$

for $d \leq 3$, this implies that $\widetilde{V}_1 (-\Delta + 1)^{-1}$ is a compact operator on $\mathfrak{H}_\Lambda$. Secondly we have also

$$\begin{aligned}
\left[\widetilde{V}_2 (-\Delta + 1)^{-1} \phi \right] (x) &= \int_\Lambda V_2(x,y) \left[(-\Delta + 1)^{-1} \phi \right] (y)\, dy \\
&= \int_\Lambda V_2(x,y) \left[\int_\Lambda \mathcal{F}^{-1} \left[\frac{1}{p^2+1} \right] (z-y) \phi(z) dz \right] dy \\
&= \int_\Lambda \int_\Lambda V_2(x,y)\, \mathcal{F}^{-1} \left[\frac{1}{p^2+1} \right] (z-y) \phi(z) dz\, dy.
\end{aligned}$$

Thus, $\widetilde{V}_2 (-\Delta + 1)^{-1}$ is an integral operator with kernel

$$\left[\widetilde{V}_2 (-\Delta + 1)^{-1} \right] (x,z) = \int_\Lambda V_2(x,y)\, \mathcal{F}^{-1} \left[\frac{1}{p^2+1} \right] (z-y)\, dy.$$

This yields

$$\begin{aligned}
&\int_\Lambda \int_\Lambda \left| \left[\widetilde{V}_2 (-\Delta + 1)^{-1} \right] (x,z) \right|^2 dx\, dz \\
&= \int_\Lambda \int_\Lambda \left| \int_\Lambda V_2(x,y)\, \mathcal{F}^{-1} \left[\frac{1}{p^2+1} \right] (z-y) dy \right|^2 dx\, dz \\
&\leq \int_\Lambda \int_\Lambda \int_\Lambda V_2(x,y)^2 \left| \mathcal{F}^{-1} \left[\frac{1}{p^2+1} \right] (z-y) \right|^2 dx\, dz\, dy \\
&= \left(\int_\Lambda \int_\Lambda V_2(x,y)^2 dx\, dy \right) \left(\int_\Lambda \left| \mathcal{F}^{-1} \left[\frac{1}{p^2+1} \right] (z) \right|^2 dz \right).
\end{aligned}$$

But

$$\int_\Lambda \int_\Lambda V_2(x,y)^2 dx dy = \int_\Lambda \int_\Lambda W(x-y)^2 \left| \gamma(x,y) \right|^2 dx\, dy,$$

since $\forall z \in \Lambda : |W(z)| \leq \frac{c}{d_\Lambda(z)}$ for a suitable constant c and $|\gamma(x,y)|^2 \leq \gamma(x,x)\gamma(y,y)$ by the Cauchy-Schwarz inequality, then

$$\begin{aligned}\int_\Lambda \int_\Lambda V_2(x,y)^2 \, dx \, dy &\leq c^2 \int_\Lambda \int_\Lambda \frac{|\gamma(x,y)|^2}{d_\Lambda(x-y)^2} \, dx \, dy \\ &\leq c^2 \int_\Lambda \int_\Lambda \frac{\rho_\gamma(x)\rho_\gamma(y)}{d_\Lambda(x-y)^2} \, dx \, dy.\end{aligned}$$

Now fix some non-negative cut-off function χ on Λ and let $R < \frac{L}{2}$, then the function $d_\Lambda(z)^{-1} \chi\left(\frac{d_\Lambda(z)}{R}\right)$ has a unique extension by 0 in $\mathbb{R}^d$. We have by Hardy's inequality [6] for $d \neq 2$ that

$$|x|^{-2} \leq \frac{4}{(d-2)^2} (-\Delta).$$

Therefore according to the definition of the metric d_Λ on Λ, we obtain

$$\begin{aligned}\int_\Lambda \int_\Lambda \frac{\rho_\gamma(x)\rho_\gamma(y)}{d_\Lambda(x-y)^2} dx dy &\leq \int_{\mathbb{R}^d} dx \int_\Lambda \frac{\chi^2\left(\frac{|x|}{R}\right)\rho_\gamma(x)\rho_\gamma(y)}{|x-y|^2} dy \\ &\leq \frac{4}{(d-2)^2} \|\rho_\gamma\|_{L^1(\Lambda)} \int_{\mathbb{R}^d} dx \left| \nabla \left(\chi\left(\frac{|\cdot|}{R}\right) \sqrt{\rho_\gamma} \right)(x) \right|^2 \\ &\leq C \|\rho_\gamma\|_{L^1(\Lambda)} \left(\int_\Lambda \left| \left(\nabla \sqrt{\rho_\gamma}\right)(x) \right|^2 dx + \int_\Lambda \rho_\gamma(x) dx \right) < \infty,\end{aligned}$$

since the kinetic energy $\operatorname{Tr}\{-\Delta\gamma\}$ is assumed to be finite. This implies

$$\begin{aligned}&\int_\Lambda \int_\Lambda \left| \left[\widetilde{V}_1 (-\Delta + 1)^{-1} \right](x,y) \right|^2 \, dx \, dy \\ &\leq C_1 \|\rho_\gamma\|_{L^1(\Lambda)} \left(\int_\Lambda \left| \left(\nabla \sqrt{\rho_\gamma}\right)(x) \right|^2 dx + N \right) \left\| \left(p^2+1\right)^{-1} \right\|_{\ell^2\left[(L\mathbb{Z})^d\right]},\end{aligned}$$

is finite for $d \leq 3$, where $C_1 = C \cdot c^2$ and shows that $\widetilde{V}_2 (-\Delta + 1)^{-1}$ is a compact operator on $\mathfrak{H}_\Lambda$. By Weyl's theorem is $\sigma_{\text{ess}}(-\Delta) = \sigma_{\text{ess}}\left(H_{\text{eff}}^{(g)}\right)$. But $-\Delta$ is defined on bounded domain Λ, hence $-\Delta$ has purely discrete spectrum, i.e., $\sigma_{\text{ess}}(-\Delta) = \emptyset$. Further, it is known that $-\Delta$ is bounded below by 0, therefore the Kato-Rellich theorem implies that $H_{\text{eff}}^{(g)}(\gamma)$ is self-adjoint and bounded below by $-\max\left\{0, \frac{b}{1-a}\right\}$ with a, b is the sum of the relative bounds for the potential V and the operator $\widetilde{V}$ defined in (2.20) with respect to $-\Delta$. Here we have used the fact that relative compactness implies relative boundedness with zero relative bound. $\square$

Now we turn to prove Theorem 2.3 which claims that a minimizer γ_{per} of the HF functional $\mathcal{E}_{\text{hf}}$ is a projection onto the lowest N eigenvalues of the effective Hamiltonian $H_{\text{eff}}^{(g)}(\gamma_{\text{per}})$.

Proof of Theorem 2.3 We show that γ_{per} satisfies the self-consistent equation for $N \in \mathbb{N}$

$$\gamma_{\text{per}} = \mathbb{1}_N \left[H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) \right],$$

where $\mathbb{1}_k\Big[H_{\text{eff}}^{(g)}\Big(\gamma_{\text{per}}\Big)\Big]$ denotes the projection onto the k lowest eigenvalues of $H_{\text{eff}}^{(g)}\Big(\gamma_{\text{per}}\Big)$. Let $\gamma_{\text{per}} \in P_{\text{per}}^{(N)}$ be a minimizer of the HF functional $\mathcal{E}_{\text{hf}}$ and $0 \le \gamma_1 \le \mathbb{1}$ be some other 1-pdm on $\mathfrak{H}_\Lambda$ of trace N. We set

$$\gamma_\lambda := \gamma_{\text{per}} + \lambda\Big(\gamma_1 - \gamma_{\text{per}}\Big).$$

It is clear that $0 \le \gamma_\lambda \le \mathbb{1}$ is a 1-pdm on $\mathfrak{H}_\Lambda$ of trace N for all $\lambda \in]0,1]$. Moreover,

$$\mathcal{E}_{\text{hf}}(\gamma_\lambda) - \mathcal{E}_{\text{hf}}(\gamma_{\text{per}}) = T(\gamma_\lambda) - T(\gamma_{\text{per}}) + \frac{g}{2}\left[Q(\gamma_\lambda,\gamma_\lambda) - Q(\gamma_{\text{per}},\gamma_{\text{per}})\right],$$

where according to (1.16) we have

$$Q(\gamma_\lambda,\gamma_\lambda) = \int_\Lambda\int_\Lambda \Big\{\gamma_\lambda(x,x)\gamma_\lambda(y,y) - |\gamma_\lambda(x,y)|^2\Big\} W(x-y)dxdy.$$

An easy computation now gives

$$\begin{aligned}\gamma_\lambda(x,x)\gamma_\lambda(y,y) &= (1-\lambda)^2\gamma_{\text{per}}(x,x)\gamma_{\text{per}}(y,y) + \lambda^2\gamma_1(x,x)\gamma_1(y,y)\\ &\quad + \lambda(1-\lambda)\left[\gamma_{\text{per}}(x,x)\gamma_1(y,y) + \gamma_1(x,x)\gamma_{\text{per}}(y,y)\right]\\ |\gamma_\lambda(x,y)|^2 &= (1-\lambda)^2\left|\gamma_{\text{per}}(x,y)\right|^2 + \lambda^2\left|\gamma_1(x,y)\right|^2\\ &\quad + \lambda(1-\lambda)\left[\gamma_{\text{per}}(x,y)\overline{\gamma_1(x,y)} + \gamma_1(x,y)\overline{\gamma_{\text{per}}(x,y)}\right]. \end{aligned} \tag{2.21}$$

Since the value of the integral does not depend on the variable of integration, we get

$$\mathcal{E}_{\text{hf}}(\gamma_\lambda) - \mathcal{E}_{\text{hf}}(\gamma_{\text{per}}) = \lambda \mathrm{Tr}_{L^2(\Lambda)}\Big\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})(\gamma_1-\gamma_{\text{per}})\Big\} + \frac{g\,\lambda^2}{2}Q\left[\gamma_1-\gamma_{\text{per}},\gamma_1-\gamma_{\text{per}}\right],$$

where the effective Hamiltonian is given by

$$\left[H_{\text{eff}}^{(g)}\left(\gamma_{\text{per}}\right)\psi\right](x) = \left[h\psi\right](x) + g\int_\Lambda \Big\{\overline{\gamma_{\text{per}}(y,y)}\psi(x) - \overline{\gamma_{\text{per}}(x,y)}\psi(y)\Big\} W(x-y)dy.$$

Taking the (left-)derivative with respect to λ and passing to the limit $\lambda \longrightarrow 0$ we obtain

$$\frac{\partial}{\partial\lambda}\left[\mathcal{E}_{\text{hf}}(\gamma_\lambda) - \mathcal{E}_{\text{hf}}(\gamma_{\text{per}})\right]_{\lambda=0} = \mathrm{Tr}_{L^2(\Lambda)}\Big\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})(\gamma_1-\gamma_{\text{per}})\Big\}.$$

Since γ_{per} is a minimizer, this yields

$$\mathrm{Tr}_{L^2(\Lambda)}\left\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\gamma_{\text{per}}\right\} \leq \mathrm{Tr}_{L^2(\Lambda)}\left\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\gamma_1\right\}. \tag{2.22}$$

We now go further and use the freedom given by choosing γ_1. Therefore, let

$$\gamma_1 = \sum_{i=1}^{\infty} \lambda_i \, |\varphi_i\rangle\langle\varphi_i|,$$

where $0 \leq \lambda_i \leq 1$ with $\sum_{i=1}^{\infty} \lambda_i = N$ and $\langle\varphi_i|\varphi_j\rangle = \delta_{i,j}$. Moreover, the Hamiltonian $H_{\text{eff}}^{(g)}(\gamma_{\text{per}})$ is a self-adjoint operator on $\mathfrak{H}_\Lambda$ whose spectrum is purely discrete, hence there exists a set $\{e_i\}_{i\in\mathbb{N}}$ in $\mathbb{R}$ with $e_1 \leq e_2 \leq \ldots$ and an orthonormal set of vectors $\{\psi_i\}_{i\in\mathbb{N}}$ such that

$$H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) = \sum_{i=1}^{\infty} e_i \, |\psi_i\rangle\langle\psi_i|.$$

Thus,

$$\mathrm{Tr}\left\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\,\gamma_1\right\} = \sum_{i,j=1}^{\infty} \lambda_j \, e_i \, |\langle\psi_i|\varphi_j\rangle|^2.$$

Using the positivity of λ_i for every $i \in \mathbb{N}$ and Cauchy-Schwarz inequality we obtain that

$$\mathrm{Tr}\left\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\,\gamma_1\right\} \geq \sum_{i=1}^{N} e_i = \mathrm{Tr}\left\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\,\mathbb{1}\left[H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) \leq e_N\right]\right\}.$$

According to (2.22) by choosing $\gamma_1 = \mathbb{1}\left[H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) \leq e_N\right]$ we get on the one hand

$$\mathrm{Tr}\left\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\,\gamma_{\text{per}}\right\} \leq \mathrm{Tr}\left\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\,\mathbb{1}\left[H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) \leq e_N\right]\right\}. \tag{2.23}$$

On the other hand we have again

$$\mathrm{Tr}\left\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\,\gamma_{\text{per}}\right\} \geq \sum_{i=1}^{N} e_i.$$

We obtain also an equality in (2.23). Since the pair-interaction potential W is positive and shells are always closed in HF theory as shown in Lemma 2.5 below, this implies that there is a gap above the N^{th} energy level, thus

$$\gamma_{per} = \mathbb{1}\left[H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) \leq e_N\right].$$

□

The existence of a gap in the spectrum of $H_{\text{eff}}^{(g)}$ is nothing but a consequence of the fact that shells are always closed in HF Theory [34], whose proof is repeated below.

Lemma 2.5. *Assume that W is positive definite, i.e., for every nonzero function $\varphi \in \mathfrak{H}_\Lambda \times \mathfrak{H}_\Lambda$ we have*

$$\langle \varphi | W \varphi \rangle = \int_\Lambda |\varphi(x,y)|^2 \, W(x,y)\, dx\, dy \; > 0$$

Let ψ be an eigenfunction of $H_{\text{eff}}^{(g)}$ defined in (2.1) *with eigenvalue e that is orthogonal to the minimizing set $\psi_1, \dots, \psi_N$. Then $e > e_i$ for all $1 \le i \le N$, i.e., the spectrum of the Hamiltonian $H_{\text{eff}}^{(g)}(\gamma)$ has a gap above the energy level number N.*

Proof. For notational convenience we assume $e_1 \le e_2 \le \ldots \le e_N$ and denote e by e_{N+1} and its corresponding eigenfunction by ψ_{N+1}. A proof by contradiction to the assumption $e_{N+1} \le e_N$ will be presented. Now, for $\lambda \in [0,1]$ we consider

$$\begin{aligned} \gamma_\lambda : &= \gamma_{\text{per}} + \lambda \gamma_1 \\ &:= \sum_{k=1}^{N-1} |\psi_k\rangle\langle\psi_k| + \Big\{ (1-\lambda)|\psi_N\rangle\langle\psi_N| + \lambda|\psi_{N+1}\rangle\langle\psi_{N+1}| \Big\}, \end{aligned}$$

i.e.,

$$\gamma_1 = -|\psi_N\rangle\langle\psi_N| + |\psi_{N+1}\rangle\langle\psi_{N+1}|.$$

Then $0 \le \gamma_\lambda \le \mathbb{1}$, $\mathrm{Tr}_{L^2(\Lambda)}(\gamma_\lambda) = N$ and $\gamma_\lambda \in \mathscr{L}^1(\mathfrak{H}_\Lambda)$. By a similar calculation as in (2.21) we have

$$\begin{aligned} \mathcal{E}_{\text{hf}}(\gamma_\lambda) - \mathcal{E}_{\text{hf}}(\gamma_{\text{per}}) &= \mathrm{Tr}_{L^2(\Lambda)} \Big\{ H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\,(\gamma_\lambda - \gamma_{\text{per}}) \Big\} + \frac{g}{2} \Big\{ Q[\gamma_\lambda, \gamma_\lambda] - Q[\gamma_{\text{per}}, \gamma_{\text{per}}] \Big\} \\ &= \lambda\, \mathrm{Tr}_{L^2(\Lambda)} \Big\{ H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) \gamma_1 \Big\} + \frac{g\lambda^2}{2}\, Q[\gamma_1, \gamma_1], \end{aligned}$$

where

$$Q[\eta, k] := \int_\Lambda \int_\Lambda \Big\{ \overline{\eta(x,x)} k(y,y) - \overline{\eta(x,y)} k(x,y) \Big\} W(x-y) dx dy.$$

We have

$$\mathrm{Tr}_{L^2(\Lambda)} \Big\{ H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\,(\gamma_\lambda - \gamma_{\text{per}}) \Big\} = \mathrm{Tr}_{L^2(\Lambda)} \Big\{ H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) \big(-|\psi_N\rangle\langle\psi_N| + |\varphi_1\rangle\langle\varphi_1| \big) \Big\},$$

and also

$$\begin{aligned} Q[\gamma_1, \gamma_1] = \int_\Lambda \int_\Lambda \{ &- |\psi_N(x)|^2\, |\psi_{N+1}(y)|^2 - |\psi_{N+1}(x)|^2\, |\psi_N(y)|^2 + \psi_N(x)\, \overline{\psi_N}(y) \\ &\cdot \overline{\psi_{N+1}}(x)\, \psi_{N+1}(y) + \psi_{N+1}(x)\, \overline{\psi_{N+1}}(y)\, \overline{\psi_N}(x)\, \psi_n(y) \}\, W(x-y)\, dx\, dy. \end{aligned}$$

Since $W > 0$ we notice that $Q[\gamma_1, \gamma_1] < 0$. Indeed we have

$$Q[\gamma_1, \gamma_1] = \int_\Lambda \int_\Lambda - W(x-y)\ |(\psi_N \wedge \psi_{N+1})(x,y)|^2\ dx\, dy,$$

and $\psi_N \wedge \psi_{N+1} \neq 0$ because $\|\psi_N\| = \|\psi_{N+1}\| = 1, \ \ \psi_N \perp \psi_{N+1}$. We also obtain

$$\begin{aligned} \mathcal{E}_{\mathrm{hf}}(\gamma_\lambda) - \mathcal{E}_{\mathrm{hf}}(\gamma_{\mathrm{per}}) &= \lambda(-e_N + e_{N+1}) + \frac{g, \lambda^2}{2} Q[\gamma_1, \gamma_1]. \\ &\leq \frac{g\,\lambda^2}{2} Q[\gamma_1, \gamma_1], \end{aligned}$$

The last inequality uses the assumption $e_{N+1} \leq e_N$ and $\lambda \in [0,1]$. Since $Q[\gamma_1, \gamma_1] \leq 0$ and $0 < g \ll 1$ we have then a contradiction to the minimality of γ_{per} and thus $e_N < e_{N+1}$. □

2.1.3 Uniqueness of the Periodic Minimizer

Until recently there is not a lot of works about the problem of uniqueness of solutions to the HF equations of atoms. The first work in this regard was by Catto, Le Bris and Lions [14], where they proved the uniqueness of the minimizing electronic density up to invariance properties of the HF energy functional. In 2010 Griesemer and Hantsch [11] solved the problem for a closed shell atom providing that the atomic number Z is sufficiently large compared to the number N of electrons. In the proof of the following lemma we employ the idea of Griesemer and Hantsch and introduce the uniqueness property of the periodic minimizer γ_{per} by using the contraction mapping principle and assuming a positive size for the spectral gap between the N^{th} eigenvalue of h and the rest spectrum.

Theorem 2.4. *Let $\gamma_{\mathrm{per}} \in P^{(N)}_{\mathrm{per}}$ be a minimizer for the HF functional $\mathcal{E}_{\mathrm{hf}}$ and the potential V is a symmetric and a relatively compact perturbation of $-\Delta$. Moreover suppose W be a repulsive pair interaction potential on $\mathfrak{H}_\Lambda \otimes \mathfrak{H}_\Lambda$ such that*

$$\forall z \in \Lambda : |W(z)| \leq \frac{c}{d_\Lambda(z)},$$

where $d_\Lambda : \Lambda \longrightarrow \mathbb{R}_0^+$ with $d_\Lambda(z) := \inf\Big\{|z + Lq| \,\Big|\, q \in \mathbb{Z}^d\Big\}$ defines a metric on Λ and $c < \infty$ is a suitable constant. Moreover, assume that the N^{th} eigenvalue of h is separated by a gap of size $2a$ with $a > 0$ from the rest spectrum. Then γ_{per} is the unique minimizer in $P^{(N)}_{\mathrm{per}}$, provided $g > 0$ is sufficiently small.

Before giving the proof of Theorem 2.4 we formulate two important auxiliary results. We show that the periodic minimizer for the HF functional satisfies a self-consistent equation which is used to establish its uniqueness.

Lemma 2.6. *Let $N \in \mathbb{N}$, $0 < g \ll 1$, $P_{\text{per}}^{(N)}$ defined in* (2.3) *and $\gamma_{\text{per}} \in P_{\text{per}}^{(N)}$ a minimizer of the HF functional. Assume that $W > 0$. Then there is $\mu \in \mathbb{R}$ and $\delta > 0$ such that*

$$\gamma_{\text{per}} = \mathbb{1}\left[H_{\text{eff}}^{(g)}\left(\gamma_{\text{per}}\right) < \mu - \delta\right] \text{ and } \gamma_{\text{per}}^{\perp} = \mathbb{1}\left[H_{\text{eff}}^{(g)}\left(\gamma_{\text{per}}\right) > \mu + \delta\right].$$

Proof. According to Theorem 2.3 we have

$$\gamma_{\text{per}} = \mathbb{1}\left[H_{\text{eff}}^{(g)}\left(\gamma_{\text{per}}\right) \leq e_N\right],$$

where e_N is the N^{th} eigenvalue of $H_{\text{eff}}^{(g)}\left(\gamma_{\text{per}}\right)$. Since the effective Hamiltonian has a purely discrete spectrum by Lemma 2.7 and as in [34], $e_{N+1} - e_N \geq W_{N,N+1} > 0$, where

$$W_{N,N+1} := \langle \varphi_{N+1} \wedge \varphi_N | W\left(\varphi_{N+1} \wedge \varphi_N\right)\rangle,$$

with φ_i are the eigenfunctions of $H_{\text{eff}}^{(g)}\left(\gamma_{\text{per}}\right)$ corresponding to the eigenvalues e_i, $i \in \{N, N+1\}$, there is $\delta > 0$ and $\mu \in \mathbb{R}$ (e.g. $\mu := \frac{1}{2}(e_{N+1}+e_N)$, $\delta := \frac{1}{3}(e_{N+1}-e_N)$) such that $e_N < \mu - \delta$. □

Another property will be needed to prove Theorem 2.4.

Lemma 2.7. *Let $\mathfrak{H}$ be a Hilbert space and $(A, \mathbb{D})$, $(B, \mathbb{D})$ be two self-adjoint operators which are bounded from below. If $A \geq B$, then for all $\lambda \in \mathbb{R}$*

$$\textit{dim Ran } \mathbb{1}[B < \lambda] \geq \textit{dim Ran } \mathbb{1}[A < \lambda], \tag{2.24}$$

where, possibly, the left side or both left and right side in (2.24) *are infinite.*

Proof. Let

$$\mu_n\left(B\right) := \sup\left\{U_{B,n-1}\left(\phi_1, \ldots, \phi_{n-1}\right) \middle| \phi_1, \ldots, \phi_{n-1} \in \mathfrak{H}\right\},$$

with

$$U_{B,n}\left(\phi_1, \ldots, \phi_n\right) = \inf\left\{\langle \psi \mid B\psi \rangle \middle| \psi \in \mathbb{D}, \|\psi\| = 1, \psi \perp \{\phi_1, \ldots, \phi_n\}\right\}.$$

Since $A \geq B$, it is clearly $\mu_n\left(A\right) \geq \mu_n\left(B\right)$. Assume for all $\lambda \in \mathbb{R}$ that

$$\mu_n\left(B\right) > \lambda \text{ and } \dim \text{Ran } \mathbb{1}[B < \lambda] < \dim \text{Ran } \mathbb{1}[A < \lambda],$$

then there is at least $n := \dim \operatorname{Ran} \mathbb{1}[B < \lambda]$ orthonormal eigenvectors $\psi_1, \ldots, \psi_n \subseteq \mathbb{D}$, $\langle \psi_i | \psi_j \rangle = \delta_{i,j}$ with eigenvalues $e_1, \ldots, e_n < \lambda < \mu_n(A)$.
Let $\psi \in X := \operatorname{span}\{\psi_1, \ldots, \psi_n\}$, i.e., $\psi = \sum_{i=1}^{n} c_i \psi_i$, then

$$\begin{aligned}\langle \psi | A\psi \rangle &= \left\langle \sum_{i=1}^{n} c_i \psi_i \middle| \sum_{j=1}^{n} c_j A\psi_j \right\rangle \\ &= \sum_{i=1}^{n} |c_i|^2 e_i < \sum_{i=1}^{n} |c_i|^2 \lambda = \lambda \|\psi\|^2 .\end{aligned}$$

Now let $\phi_1, \ldots, \phi_{n-1} \in \mathfrak{H}$, then there is always $\psi \in X \cap \{\phi_1, \ldots, \phi_{n-1}\}^{\perp}$ with $\|\psi\| = 1$ such that

$$U_{A,n-1}(\phi_1, \ldots, \phi_{n-1}) \leq \langle \psi \mid A\psi \rangle < \lambda.$$

Thus,

$$\mu_n(A) := \sup\Big\{ U_{A,n-1}(\phi_1, \ldots, \phi_{n-1}) \,\Big|\, \phi_1, \ldots, \phi_{n-1} \in \mathfrak{H} \Big\} < \lambda,$$

which contradicts $\mu_n(A) > \lambda$. □

Proof of Theorem 2.4: We use the contraction mapping principle to prove the uniqueness of γ_{per} in $P_{\mathrm{per}}^{(N)}$. We define therefore the function

$$\begin{aligned}F_g : &D \subset \mathscr{L}^1(\mathfrak{H}_\Lambda) \longrightarrow \mathscr{L}^1(\mathfrak{H}_\Lambda) \\ &\gamma \longmapsto F_g(\gamma) = \mathbb{1}[H_{\mathrm{eff}}^{(g)}(\gamma) < \mu].\end{aligned}$$

where $\mu \in \mathbb{R}$ and

$$D = \Big\{ \gamma = \gamma^* = \gamma^2 \mid \operatorname{Tr}_{L^2(\Lambda)}(\gamma) < \infty \Big\}.$$

is the set of orthogonal projections with finite trace. We must show

1. $D \subseteq \mathscr{L}^1(\mathfrak{H}_\Lambda)$ is complete with respect to the metric

   $$d(\gamma, \gamma') = \|\gamma - \gamma'\|_{\mathscr{L}^1},$$

2. F_g is well-defined, i.e., for all $\gamma \in D$: $\dim \operatorname{Ran}(F_g) < \infty$ and $F_g(D) \subseteq D$,

3. $F_g \mathbb{1}_D$ is a contraction with respect to the Hilbert-Schmidt norm, i.e., $\forall \gamma, \gamma_{\mathrm{per}} \in D$, $\exists\ 0 \leq M < 1$ such that

   $$\|F_g(\gamma) - F_g(\gamma_{\mathrm{per}})\|_{HS} \leq M \|\gamma - \gamma_{\mathrm{per}}\|_{HS} . \tag{2.25}$$

Since the space of trace class operators is complete, it is enough to show that D is closed. For this purpose let $\{\gamma_n\}_{n\in I} \subseteq D$ be a net in D which converges to $\gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda)$. We must show that $\gamma \in D$. First we prove that $\gamma = \gamma^*$, by the triangle inequality we have

$$\|\gamma - \gamma^*\|_{\mathscr{L}^1} \leq \|\gamma - \gamma_n\|_{\mathscr{L}^1} + \|\gamma_n - \gamma^*\|_{\mathscr{L}^1}.$$

Since $\{\gamma_n\}_{n\in I} \longrightarrow \gamma$ as $n \longrightarrow \infty$, it remains to show that $\|\gamma_n - \gamma^*\|_{\mathscr{L}^1} \longrightarrow 0$. Since $\gamma_n \in D$, we have: $\forall n \in I, \gamma_n = \gamma_n^*$, and because of the anti-linearity of $*$ we get

$$\|\gamma_n - \gamma^*\|_{\mathscr{L}^1} = \|\gamma_n^* - \gamma^*\|_{\mathscr{L}^1} = \left\|(\gamma_n - \gamma)^*\right\|_{\mathscr{L}^1} = \|\gamma_n - \gamma\|_{\mathscr{L}^1},$$

where the last equation is satisfied, since $(\gamma_n - \gamma)^*$ and $\gamma_n - \gamma$ have the same singular values. Moreover, since $\mathrm{Tr}_{L^2(\Lambda)}(\gamma_n) < \infty$, we have

$$\left|\mathrm{Tr}_{L^2(\Lambda)}(\gamma_n) - \mathrm{Tr}_{L^2(\Lambda)}(\gamma)\right| = \left|\mathrm{Tr}_{L^2(\Lambda)}(\gamma_n - \gamma)\right| \leq \mathrm{Tr}_{L^2(\Lambda)}|\gamma_n - \gamma|.$$

Therefore

$$\mathrm{Tr}_{L^2(\Lambda)}(\gamma) < \infty. \tag{2.26}$$

We also get $\gamma = \gamma^2$ when $\|\gamma_n - \gamma^2\|_{\mathscr{L}^1} \longrightarrow 0$. Indeed,

$$\left\|\gamma_n - \gamma^2\right\|_{\mathscr{L}^1} = \left\|\gamma_n^2 - \gamma^2\right\|_{\mathscr{L}^1} \leq \left[\|\gamma_n\|_{op} + \|\gamma\|_{op}\right]\|\gamma_n - \gamma\|_{\mathscr{L}^1},$$

where we have used $\gamma_n = \gamma_n^2$ and $\gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda)$.
For the second claim, that F_g is well-defined, we assume that the number of the eigenvalues of $h = -\Delta + V$ below μ is finite, i.e.,

$$\sharp\Big\{\sigma(h) \cap]-\infty, \mu[\Big\} < \infty, \tag{2.27}$$

To prove that $\dim \mathrm{Ran}(F_g) < \infty$, it must be shown that (2.27) is satisfied for $H_{\mathrm{eff}}^{(g)}$. According to Lemma 2.7 we must prove that h and $H_{\mathrm{eff}}^{(g)}$ are self-adjoint operators and bounded from below, but this follows from Lemma 2.7 directly. Moreover we must also show that $H_{\mathrm{eff}}^{(g)} \geq h$. Indeed, as in [33] we introduce $\vartheta := \sqrt{\gamma}$ and $\vartheta_z(x) := \vartheta(z, x)$, so that for all $x, y \in \Lambda$, we have

$$\gamma(x, y) = \int_\Lambda \overline{\vartheta_z(x)}\,\vartheta_z(y)\,dz. \tag{2.28}$$

Further, for normalized $\varphi \in \mathfrak{H}_\Lambda$, we can write

$$\begin{aligned}\langle\varphi|\widetilde{V}\varphi\rangle &= \int_\Lambda \overline{\varphi(x)}\Big\{g\int_\Lambda \Big(\gamma(y,y) - \overline{\gamma(x,y)}\Big)W(x-y)dy\Big\}\varphi(x)dx \\ &= g\int_\Lambda \overline{\varphi(x)}\int_\Lambda \Big(\gamma(y,y)\varphi(x) - \overline{\gamma(x,y)}\varphi(y)\Big)W(x-y)dydx. \end{aligned}\tag{2.29}$$

But equation (2.28) implies

$$\langle\varphi|\widetilde{V}\varphi\rangle = g\int_\Lambda \overline{\varphi(x)}\int_\Lambda\Big(\int_\Lambda \overline{\vartheta_z(y)}\,\vartheta_z(y)\,dz\Big)\,\varphi(x)\,W(x-y)\,dy\,dx$$
$$- g\int_\Lambda \overline{\varphi(x)}\int_\Lambda\Big(\int_\Lambda \vartheta_z(x)\,\overline{\vartheta_z(y)}\,dz\Big)\,\varphi(y)\,W(x-y)\,dy\,dx,$$

which is according to Fubini's theorem equivalent to

$$\langle\varphi|\widetilde{V}\varphi\rangle = g\int_\Lambda\int_\Lambda\int_\Lambda |\varphi(x)|^2\,|\vartheta_z(y)|^2\,W(x-y)\,dz\,dy\,dx$$
$$- g\int_\Lambda\int_\Lambda\int_\Lambda \overline{\varphi(x)}\,\varphi(y)\,\vartheta_z(x)\,\overline{\vartheta_z}(y)\,\varphi(y)\,W(x-y)\,dz\,dy\,dx,$$

This, however, can be rewritten as

$$\langle\varphi|\widetilde{V}\varphi\rangle = g\int_\Lambda\Big\{\langle\varphi\otimes\vartheta_z|W(\varphi\otimes\vartheta_z)\rangle - \langle\varphi\otimes\vartheta_z|W(\vartheta_z\otimes\varphi)\rangle\Big\}dz.$$

Since $W \geq 0$ is non-negative, the Cauchy-Schwarz Inequality implies

$$\begin{aligned}&\langle\varphi\otimes\vartheta_z|W\,(\vartheta_z\otimes\varphi)\rangle \leq |\langle\varphi\otimes\vartheta_z|W\,(\vartheta_z\otimes\varphi)\rangle| \\ &\leq \langle\varphi\otimes\vartheta_z|W\,(\varphi\otimes\vartheta_z)\rangle^{1/2}\,\langle\vartheta_z\otimes\varphi|W\,(\vartheta_z\otimes\varphi)\rangle^{1/2},\end{aligned} \tag{2.30}$$

so we reach our goal, if we show the equality of the two terms on the right side of (2.30). For this purpose we note

$$\langle\varphi\otimes\vartheta_z|W\,(\varphi\otimes\vartheta_z)\rangle = \int_\Lambda\int_\Lambda \overline{\varphi(x)}\,\overline{\vartheta_z(y)}W(x-y)\varphi(x)\vartheta_z(y)dxdy.$$

Interchanging x and y gives

$$\langle\varphi\otimes\vartheta_z|W\,(\varphi\otimes\vartheta_z)\rangle = \int_\Lambda\int_\Lambda \overline{\varphi(y)}\,\overline{\vartheta_z(x)}W(y-x)\varphi(y)\vartheta_z(x)dy\,dx,$$

But the symmetry of W, $W(z) = W(-z)$, implies

$$\begin{aligned}\langle\varphi\otimes\vartheta_z|W\,(\varphi\otimes\vartheta_z)\rangle &= \int_\Lambda\int_\Lambda \overline{\varphi(y)}\,\overline{\vartheta_z(x)}W(x-y)\varphi(y)\vartheta_z(x)dy\,dx \\ &= \langle\vartheta_z\otimes\varphi|W\,(\vartheta_z\otimes\varphi)\rangle.\end{aligned}$$

Thus, the operator $\widetilde{V}$ is non-negative and by Lemma 2.7

$$\dim \mathrm{Ran}\mathbb{1}\left[H_{\mathrm{eff}}^{(g)} < \mu\right] \leq \dim \mathrm{Ran}\mathbb{1}\left[h < \mu\right] < \infty.$$

To conclude the proof of claim 2, it is necessary to show that

$$\gamma \in D \Longrightarrow F_g(\gamma) \in D.$$

Let $\gamma \in F_g(D)$. Then there is $\gamma_0 \in D$ such that $F_g(\gamma_0) = \gamma$. To show $\gamma \in D$, we must prove

1. $\gamma = \gamma^* = \gamma^2$,
2. $\mathrm{Tr}_{L^2(\Lambda)}(\gamma) < \infty$.

We remark that

$$\gamma^2 = [F_g(\gamma_0)]^2 = \left(\mathbb{1}\left[H_{\mathrm{eff}}^{(g)}(\gamma_0) < \mu\right]\right)^2 = \mathbb{1}\left[H_{\mathrm{eff}}^{(g)}(\gamma_0) < \mu\right] = \gamma,$$

since γ is a projection. Using the functional calculus for self-adjoint operators we have

$$\gamma^* = [F_g(\gamma_0)]^* = \left(\mathbb{1}\left[H_{\mathrm{eff}}^{(g)}(\gamma_0) < \mu\right]\right)^* = \mathbb{1}\left[H_{\mathrm{eff}}^{(g)}(\gamma_0) < \mu\right] = \gamma.$$

Thus point 1 is obtained. Further,

$$\begin{aligned}
\mathrm{Tr}_{L^2(\Lambda)}(\gamma) &= \mathrm{Tr}_{L^2(\Lambda)}\{F_g(\gamma_0)\} \\
&= \mathrm{Tr}_{L^2(\Lambda)}\left\{\mathbb{1}\left[H_{\mathrm{eff}}^{(g)}(\gamma_0) < \mu\right]\right\} \\
&= \dim \mathrm{Ran}\, \mathbb{1}\left[H_{\mathrm{eff}}^{(g)}(\gamma_0) < \mu\right] \\
&\leq \dim \mathrm{Ran}\, \mathbb{1}\left[h < \mu\right] < \infty.
\end{aligned}$$

To show $F_g\mathbb{1}_D$ is a contraction, we prove in Appendix B that

$$\gamma_{\mathrm{g}} = \mathbb{1}\left[H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{g}}) < \mu\right] = \frac{-1}{2\pi i}\int_{\mathbb{R}} (H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}}) - z\mathbb{1})^{-1} dz - \frac{1}{2}\mathbb{1}. \tag{2.31}$$

Therefore,

$$\begin{aligned}
&F_g(\gamma) - F_g(\gamma_{\mathrm{per}}) = \mathbb{1}\left[H_{\mathrm{eff}}^{(g)}(\gamma) < \mu\right] - \mathbb{1}\left[H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}}) < \mu\right] \\
&= (-\frac{1}{2\pi i}\int_{\mathbb{R}} (H_{\mathrm{eff}}^{(g)}(\gamma) + i\lambda)^{-1} d\lambda - \frac{1}{2}\mathbb{1}) - (-\frac{1}{2\pi i}\int_{\mathbb{R}} (H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}}) + i\lambda)^{-1} d\lambda - \frac{1}{2}\mathbb{1}).
\end{aligned} \tag{2.32}$$

Using the second resolvent equation we obtain

$$F_g(\gamma) - F_g(\gamma_{\text{per}}) = \frac{1}{2\pi i}\int_{\mathbb{R}} (H_{\text{eff}}^{(g)}(\gamma) + i\lambda)^{-1} \left(H_{\text{eff}}^{(g)}(\gamma) - H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\right) (H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) + i\lambda)^{-1} d\lambda,$$

where

$$\begin{aligned} &\left[\left(H_{\text{eff}}^{(g)}(\gamma) - H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\right)\varphi\right](x) \\ &= \frac{g}{2}\left[\left(\rho_{(\gamma-\gamma_{\text{per}})} \star W\right)\varphi\right](x) - \frac{g}{2}\int_{\Lambda} \left(\overline{\gamma - \gamma_{\text{per}}}\right)(x,y) W(x-y)\varphi(y) dy. \end{aligned}$$

Now we consider

$$X := \frac{g}{4\pi i}\int_{\mathbb{R}} (H_{\text{eff}}^{(g)}(\gamma) + i\lambda)^{-1} \left(\rho_{(\gamma-\gamma_{\text{per}})} \star W\right) (H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) + i\lambda)^{-1} d\lambda. \tag{2.33}$$

We show that X is a Hilbert-Schmidt operator by approximating it in terms of $\|\gamma - \gamma_{\text{per}}\|_{HS}$. For simplicity we denote

$$\begin{aligned} A_\lambda &:= (-\Delta + a.1 - i\lambda)^{-1} \\ B &:= \rho_{(\gamma-\gamma_{\text{per}})} \star W \\ D_\lambda &:= (H_{\text{eff}}^{(g)}(\gamma) + i\lambda)^{-1}, \end{aligned} \tag{2.34}$$

with $a \geq 0$, where the N^{th} eigenvalue of h is separated by a gap of size $2a$ from the rest of the spectrum according to the assumption. It will be shown that $A_\lambda B A_\lambda^*$ is a Hilbert-Schmidt operator. By using the Hilbert-Schmidt norm we can write

$$\|A_\lambda^* B A_\lambda\|_{HS}^2 = \operatorname{Tr}\left\{A_\lambda^* B A_\lambda A_\lambda^* B A_\lambda\right\},$$

which is equivalent to

$$\|A_\lambda^* B A_\lambda\|_{HS}^2 = \operatorname{Tr}\left\{A_\lambda A_\lambda^* B A_\lambda A_\lambda^* B\right\}$$

due to the invariance of the trace under cyclic permutations. We denote $A_\lambda A_\lambda^*$ by S, where

$$S := |A_\lambda|^2 = A_\lambda A_\lambda^* = \left((-\Delta + a)^2 + \lambda^2\right)^{-1},$$

and its kernel by $S(x-y)$. Then

$$\begin{aligned} \|A_\lambda^* B A_\lambda\|_{HS}^2 &= \int_{\Lambda}\int_{\Lambda} dx\, dy \left\{S(y,x)B(x)S(x,y)B(y)\right\} \\ &= \int_{\Lambda}\int_{\Lambda} dx\, dy\, B(x)B(y)\left|S(x-y)\right|^2. \end{aligned}$$

Substituting B as in (2.34) we get

$$\begin{aligned}\|A_\lambda^* B A_\lambda\|_{HS}^2 &= \int\limits_\Lambda\int\limits_\Lambda\int\limits_\Lambda\int\limits_\Lambda dx\,dy\,du\,dv\,|S(x-y)|^2\,W(x-u)\rho_{(\gamma-\gamma_{\rm per})}(u)W(y-v)\rho_{(\gamma-\gamma_{\rm per})}(v)\\ &\le \|\rho_{(\gamma-\gamma_{\rm per})}\|_{L^1(\Lambda)}^2 \sup_{u,v}\int\limits_\Lambda\int\limits_\Lambda dx\,dy\,|S(x-y)|^2\,|\overline{W}(x-u)|\,|W(y-v)|.\end{aligned}$$

Setting $\varphi_u(x) := W(x-u)$, we note that, since $|S|$ is bounded and self-adjoint and $W(\cdot)\in L^2(\Lambda)$, the last inequality can be written as

$$\begin{aligned}\|A_\lambda^* B A_\lambda\|_{HS}^2 &\le \left\|\rho_{(\gamma-\gamma_{\rm per})}\right\|_{L^1(\Lambda)}^2 \sup_{u,v}\,\langle\varphi_u\big||S|^2\star\varphi_v\rangle\\ &= \left\|\rho_{(\gamma-\gamma_{\rm per})}\right\|_{L^1(\Lambda)}^2 \sup_{u,v}\,\langle|S|\star\varphi_u\big||S|\star\varphi_v\rangle.\end{aligned}$$

Using the Cauchy-Schwarz Inequality gives

$$\|A_\lambda^* B A_\lambda\|_{HS}^2 \le \left\|\rho_{(\gamma-\gamma_{\rm per})}\right\|_{L^1(\Lambda)}^2 \sup_u\,\||S|\star\varphi_u\|_{L^2(\Lambda)}^2\,.$$

Now, the Plancherel theorem leads to

$$\|A_\lambda^* B A_\lambda\|_{HS}^2 \le \left\|\rho_{(\gamma-\gamma_{\rm per})}\right\|_{L^1(\Lambda)}^2 \sup_u\,\left\{\|\mathscr{F}(|S|\star\varphi_u)\|_{L^2(\Lambda)}^2\right\}.$$

But

$$\begin{aligned}\mathscr{F}(|S|\star\varphi_u) &= |\Lambda|^{-\frac12}\,\mathscr{F}(|S|)\mathscr{F}(\varphi_u)\\ &= |\Lambda|^{-\frac12}\,e^{i\xi u}\mathscr{F}(|S|)\mathscr{F}(\varphi_0).\end{aligned}$$

This implies

$$\|A_\lambda^* B A_\lambda\|_{HS}^2 \le |\Lambda|^{-1}\left\|\rho_{(\gamma-\gamma_{\rm per})}\right\|_{L^1(\Lambda)}^2 \|\mathscr{F}(|S|)\mathscr{F}(\varphi_0)\|_{L^2(\Lambda)}^2\,.$$

For the estimate on $\left\|\rho_{(\gamma-\gamma_{\rm per})}\right\|_{L^1(\Lambda)}^2$, we first note that

$$\begin{aligned}\left\|\rho_{(\gamma-\gamma_{\rm per})}\right\|_{L^1(\Lambda)} &= \int\limits_\Lambda \left|\rho_{(\gamma-\gamma_{\rm per})}(x)\right| dx\\ &= \int\limits_\Lambda \left|(\gamma-\gamma_{\rm per})(x,x)\right| dx.\end{aligned}$$

But $\gamma(x,x) = \int\limits_\Lambda |\gamma^{\frac{1}{2}}(x,y)|^2 dy$, which gives

$$\begin{aligned}\left\|\rho_{(\gamma-\gamma_{\text{per}})}\right\|_{L^1(\Lambda)} &= \int\limits_\Lambda \left| \int\limits_\Lambda \left|\gamma^{\frac{1}{2}}(x,y)\right|^2 - \left|\gamma_{\text{per}}^{\frac{1}{2}}(x,y)\right|^2 dy \right| dx \\ &= \int\limits_\Lambda \left| \int\limits_\Lambda \left(\overline{\gamma}^{\frac{1}{2}} + \overline{\gamma}_{\text{per}}^{\frac{1}{2}}\right)(x,y) \left(\gamma^{\frac{1}{2}} - \gamma_{\text{per}}^{\frac{1}{2}}\right)(x,y) dy \right| dx.\end{aligned}$$

Applying the Cauchy-Schwarz Inequality with respect to y and then to x gives

$$\begin{aligned}&\left\|\rho_{(\gamma-\gamma_{\text{per}})}\right\|_{L^1(\Lambda)} \\ &\leq \int\limits_\Lambda (\int\limits_\Lambda \left|(\overline{\gamma}^{\frac{1}{2}} + \overline{\gamma}_{\text{per}}^{\frac{1}{2}})(x,y)\right|^2 dy)^{\frac{1}{2}} (\int\limits_\Lambda \left|\left(\gamma^{\frac{1}{2}} - \gamma_{\text{per}}^{\frac{1}{2}}\right)(x,y)\right|^2 dy)^{\frac{1}{2}} dx \\ &\leq (\int\limits_\Lambda\int\limits_\Lambda \left|(\overline{\gamma}^{\frac{1}{2}} + \overline{\gamma}_{\text{per}}^{\frac{1}{2}})(x,y)\right|^2 dydx)^{\frac{1}{2}} (\int\limits_\Lambda\int\limits_\Lambda \left|(\gamma^{\frac{1}{2}} - \gamma_{\text{per}}^{\frac{1}{2}})(x,y)\right|^2 dydx)^{\frac{1}{2}} \\ &\leq \left\|\overline{\gamma}^{\frac{1}{2}} + \overline{\gamma}_{\text{per}}^{\frac{1}{2}}\right\|_{HS} \cdot \left\|\gamma^{\frac{1}{2}} - \gamma_{\text{per}}^{\frac{1}{2}}\right\|_{HS}.\end{aligned}$$

Since γ and γ_{per} are projections,

$$\left\|\rho_{(\gamma-\gamma_{\text{per}})}\right\|_{L^1(\Lambda)} \leq \|\gamma - \gamma_{\text{per}}\|_{HS} \cdot \left\|\overline{\gamma} + \overline{\gamma}_{\text{per}}\right\|_{HS}.$$

To verify that $A_\lambda B A_\lambda^*$ is a Hilbert-Schmidt operator, it remains to calculate $\mathscr{F}(|S|)$, which in fact gives a constant term. We remark that

$$\begin{aligned}|S| &= |A_\lambda|^2 \\ &= \left((-\Delta + a)^2 + \lambda^2\right)^{-1} \\ &= \mathscr{F}^{-1}\left(\frac{1}{(p^2+a)^2+\lambda^2}\right).\end{aligned}$$

Therefore,

$$\begin{aligned}\mathscr{F}(|S|) &= \mathscr{F}\left[\mathscr{F}^{-1}\left(\frac{1}{(p^2+a)^2+\lambda^2}\right)\right], \\ &= \frac{1}{(p^2+a)^2+\lambda^2}.\end{aligned}$$

These estimates lead to

$$\|A_\lambda^* B A_\lambda\|_{HS} \leq \frac{1}{\sqrt{|\Lambda|}} \left\|\frac{1}{(p^2+a)^2+\lambda^2}\right\|_{L^\infty(\Lambda)} \|\gamma + \gamma_{\text{per}}\|_{HS} \|\mathcal{F}(\varphi_0)\|_{L^2(\Lambda)} \|\gamma - \gamma_{\text{per}}\|_{HS}.$$

Thus, $A_\lambda B A_\lambda^*$ is a Hilbert-Schmidt operator and (2.33) can be estimated as follows

$$\left\| X \right\|_{HS} \leq \frac{g}{4\pi} \sup_{\lambda\in\mathbb{R}} \left\{ \left\| D_\lambda A_\lambda^{-1} \right\|_{op} \left\| D_\lambda \left(A_\lambda^{-1} \right)^* \right\|_{op} \right\} \int_{\mathbb{R}} \left\| A_\lambda B A_\lambda^* \right\|_{HS} d\lambda,$$

where

$$\begin{aligned} \int_{\mathbb{R}} \left\| A_\lambda B A_\lambda^* \right\|_{HS} d\lambda &\leq \frac{1}{\sqrt{|\Lambda|}} \left\| \gamma + \gamma_{\mathrm{per}} \right\|_{HS} \left\| W \right\|_{L^2(\Lambda)} \left\| \gamma - \gamma_{\mathrm{per}} \right\|_{HS} \int_{-\infty}^{+\infty} \frac{d\lambda}{a^2 + \lambda^2} \\ &\leq \frac{\pi}{a\sqrt{|\Lambda|}} \left\| \gamma + \gamma_{\mathrm{per}} \right\|_{HS} \left\| W \right\|_{L^2(\Lambda)} \left\| \gamma - \gamma_{\mathrm{per}} \right\|_{HS}. \end{aligned}$$

Hence,

$$\left\| X \right\|_{HS} \leq \frac{gC_1}{4\pi} \sup_{\lambda\in\mathbb{R}} \left\{ \left\| D_\lambda A_\lambda^{-1} \right\|_{op} \left\| D_\lambda \left(A_\lambda^{-1} \right)^* \right\|_{op} \right\} \left\| \gamma - \gamma_{\mathrm{per}} \right\|_{HS},$$

where

$$C_1 := \frac{\pi}{a\sqrt{|\Lambda|}} \left\| W \right\|_{L^2(\Lambda)} \left\| \gamma + \gamma_{\mathrm{per}} \right\|_{HS}.$$

Moreover, the operator

$$D_\lambda A_\lambda^{-1} = \frac{1}{H_{\mathrm{eff}}^{(g)}(\gamma) + i\lambda} (-\Delta + a.1 + i\lambda)$$

is uniformly bounded with respect to $a > 0$ and $\lambda \in \mathbb{R}$. Indeed,

$$\left\| (-\Delta + W + i\lambda) A_\lambda \psi \right\|_{L^2(\Lambda)} \geq \left\| -\Delta A_\lambda \psi \right\|_{L^2(\Lambda)} - \left\| W A_\lambda \psi \right\|_{L^2(\Lambda)} - |\lambda| \left\| A_\lambda \psi \right\|_{L^2(\Lambda)}.$$

Since $W := V + g\widetilde{V}(x)$ is $-\Delta$-bounded with relative bound strictly smaller than 1, we obtain

$$\left\| W A_\lambda \psi \right\|_{L^2(\Lambda)} \leq \alpha \left\| -\Delta A_\lambda \psi \right\|_{L^2(\Lambda)} + \beta \left\| A_\lambda \psi \right\|_{L^2(\Lambda)},$$

where $\alpha < 1$ and $\beta = \beta(\alpha) < \infty$. Therefore, we have

$$\begin{aligned} &\left\| (-\Delta + W + i\lambda) A_\lambda \psi \right\|_{L^2(\Lambda)} \\ &\geq (1-\alpha) \left\| -\Delta A_\lambda \psi \right\|_{L^2(\Lambda)} - (\beta + |\lambda|) \left\| A_\lambda \psi \right\|_{L^2(\Lambda)} \\ &\geq (1-\alpha) \left\| \psi \right\|_{L^2(\Lambda)} - \left(\beta + |\lambda| + \sqrt{a^2 + \lambda^2}(1-\alpha) \right) \left\| A_\lambda \psi \right\|_{L^2(\Lambda)}. \end{aligned}$$

Since

$$\sigma\left(H_{\mathrm{eff}}^{(g)} \right) \cap [-a, a] = \emptyset \text{ for } a > 0,$$

then according to the spectral theorem we get

$$\left\|(-\Delta+W+i\lambda)^{-1}\right\|_{op}\leq\frac{1}{\operatorname{dist}\left(\lambda,\sigma\left(H_{\text{eff}}^{(g)}\right)\right)},$$

Thus, for each $\psi\in\mathfrak{H}_\Lambda$

$$\|A_\lambda\psi\|_{L^2(\Lambda)}\leq\left\|\frac{(-\Delta+W+i\lambda)}{a}A_\lambda\psi\right\|_{L^2(\Lambda)}.$$

In turn this implies

$$\begin{aligned}&\|(-\Delta+W+i\lambda)\,A_\lambda\psi\|_{L^2(\Lambda)}\\&\geq(1-\alpha)\,\|\psi\|_{L^2(\Lambda)}-\left(\frac{\beta+|\lambda|+\sqrt{a^2+\lambda^2}(1-\alpha)}{a}\right)\|(-\Delta+W+i\lambda)\,A_\lambda\psi\|_{L^2(\Lambda)},\end{aligned}$$

which is equivalent to

$$\|(-\Delta+W+i\lambda)\,A_\lambda\psi\|_{L^2(\Lambda)}\geq\frac{a(1-\alpha)}{a+\beta+|\lambda|+\sqrt{a^2+\lambda^2}(1-\alpha)}\,\|\psi\|_{L^2(\Lambda)}.$$

Hence,

$$\left\|A_\lambda^{-1}\,(-\Delta+W+i\lambda)^{-1}\right\|_{op}\leq\frac{a+\beta+|\lambda|+\sqrt{a^2+\lambda^2}(1-\alpha)}{a(1-\alpha)}<\infty.$$

The operator

$$\phi:\lambda\longmapsto\frac{-\Delta+a.1-i\lambda}{-\Delta+a.1+i\lambda}$$

is unitary, therefore

$$D_\lambda\left(A_\lambda^{-1}\right)^*=\frac{1}{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})+i\lambda}(-\Delta+a.1-i\lambda)$$

is also a uniformly bounded operator with respect to $a>0$ and $\lambda\in\mathbb{R}$.
We also have

$$\sup_\lambda\left\{\left\|D_\lambda A_\lambda^{-1}\right\|_{op}\left\|D_\lambda\left(A_\lambda^{-1}\right)^*\right\|_{op}\right\}<C_2<\infty.$$

Taking into account all estimates we arrive at

$$\|X\|_{HS}\leq\frac{g}{4\pi}\,C_1C_2\,\|\gamma-\gamma_{\text{per}}\|_{HS},$$

where $\frac{g}{4\pi} C_1 C_2 < 1$, since $0 < g \ll 1$ and $a > 0$. Now we consider

$$Y := -\frac{g}{4\pi i} \int_{\mathbb{R}} D_\lambda \Big\{ \int_{\Lambda} (\gamma - \gamma_{\mathrm{per}})(x,y) W(x-y) dy \Big\} D_\lambda \, d\lambda.$$

Following the same method as above we conclude that

$$\|Y\|_{HS} \leq \frac{g}{4\pi} C_2 \|W\|_{L^2(\Lambda)} \|\gamma - \gamma_{\mathrm{per}}\|_{HS} \,.$$

We also obtain

$$\|F_g(\gamma) - F_g(\gamma_{\mathrm{per}})\|_{HS} \leq \frac{g}{4\pi} C_2 \|W\|_{L^2(\Lambda)} \big(1 + \frac{\pi}{a\sqrt{|\Lambda|}} \|\gamma + \gamma_{\mathrm{per}}\|_{HS}\big) \|\gamma - \gamma_{\mathrm{per}}\|_{HS} \,,$$

where

$$\frac{g}{4\pi} C_2 \|W\|_{L^2(\Lambda)} \Big(1 + \frac{\pi}{a\sqrt{|\Lambda|}} \|\gamma + \gamma_{\mathrm{per}}\|_{HS}\Big) < 1,$$

since $0 < g \ll 1$. Thus, $F_g \mathbb{1}_D$ is a contraction, and therefore, by the contraction mapping principle the equation $F_g(\gamma_{\mathrm{per}}) = \gamma_{\mathrm{per}}$ has a unique solution $\gamma_{\mathrm{per}} \in D$. □

2.2 Equality between the Periodic HF Energy and the unrestricted HF Energy

We now compute the difference between the periodic HF energy and the unrestricted HF energy to conclude that the minimizer of the HF functional in the periodic setting is in fact a minimizer of the HF functional on all density matrices without the periodicity constraint.

Theorem 2.5. *Let $\gamma_{\mathrm{per}} \in P_{\mathrm{per}}^{(N)}$ be a minimizer of the HF functional $\mathcal{E}_{\mathrm{hf}}$ and $\gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda)$, with $\mathrm{Tr}\,(\gamma) = N$, $\gamma = \gamma^* = \gamma^2$ and $\mathrm{Tr}\{h\gamma\} < \infty$. Assume, moreover, that the external potential V is a symmetric and a relatively compact perturbation of $-\Delta$ and the pair interaction potential W satisfies*

$$\forall z \in \Lambda : |W(z)| \leq \frac{c}{d_\Lambda(z)}, \tag{2.35}$$

where $d_\Lambda : \Lambda \longrightarrow \mathbb{R}_0^+$ with $d_\Lambda(z) := \inf\Big\{|z + Lq| \Big| q \in \mathbb{Z}^d\Big\}$ defines a metric on Λ and $c < \infty$ is a suitable constant. Further, suppose that the N^{th} eigenvalue of h is separated by a gap of size $2a$ for $a > 0$ from the rest of the spectrum. Then

$$\mathcal{E}_{\mathrm{hf}}(\gamma) \geq \mathcal{E}_{\mathrm{hf}}(\gamma_{\mathrm{per}}), \tag{2.36}$$

provided $g > 0$ is sufficiently small. In particular the periodic HF energy coincides with the unrestricted HF energy.

Proof. Because of the Γ-periodicity of γ_{per} we can extend it to be defined on $\mathfrak{H}_\Lambda$ and thus $\mathcal{E}_{\text{hf}}(\gamma_{\text{per}})$ is well-defined. Set $\gamma_\lambda := (1-\lambda)\gamma_{\text{per}} + \lambda\gamma$, so $\operatorname{Tr}(\gamma_\lambda) = N$, for all $0 \leq \lambda \leq 1$. A similar computation as in Theorem 2.3 yields

$$\mathcal{E}_{\text{hf}}(\gamma_\lambda) - \mathcal{E}_{\text{hf}}(\gamma_{\text{per}}) = \lambda \operatorname{Tr}_{L^2(\Lambda)}\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})(\gamma - \gamma_{\text{per}})\} + \frac{g\lambda^2}{2} Q(\gamma - \gamma_{\text{per}}, \gamma - \gamma_{\text{per}}),$$

where Q is defined as in (1.16), namely:

$$Q(\gamma,\eta) := \int_\Lambda\int_\Lambda \left\{\overline{\gamma(x,x)}\eta(y,y) - \overline{\gamma(x,y)}\eta(y,x)\right\} W(x-y)\,dx\,dy.$$

Using Lemma 2.3 we know that γ_{per} is the projection onto the N lowest eigenvalues of the periodic effective Hamiltonian $H_{\text{eff}}^{(g)}$. Therefore γ_{per} commutes with $H_{\text{eff}}^{(g)}$. Further we note that

$$\begin{aligned} H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n &= \left(H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n\right)\gamma_{\text{per}}^\perp + \left(H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n\right)\gamma_{\text{per}} \\ &= \gamma_{\text{per}}^\perp \| H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n|\,\gamma_{\text{per}}^\perp - \gamma_{\text{per}}|H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n|\,\gamma_{\text{per}}, \end{aligned} \tag{2.37}$$

since $H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) \leq e_n$ on $\operatorname{Ran}\{\gamma_{\text{per}}\}$ and $H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) > e_n$ on $\operatorname{Ran}\left\{\gamma_{\text{per}}^\perp\right\}$ with e_n is the n^{th} eigenvalue of $H_{\text{eff}}^{(g)}(\gamma_{\text{per}})$. Therefore,

$$\begin{aligned} &\operatorname{Tr}_{L^2(\Lambda)}\left\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\,(\gamma - \gamma_{\text{per}})\right\} \\ &= \operatorname{Tr}_{L^2(\Lambda)}\left\{\left(H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n\right)(\gamma - \gamma_{\text{per}})\right\} \\ &= \operatorname{Tr}_{L^2(\Lambda)}\left\{\left(H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n\right)\gamma\right\} - \operatorname{Tr}_{L^2(\Lambda)}\left\{\left(H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n\right)\gamma_{\text{per}}\right\}. \end{aligned}$$

Using (2.37) we obtain

$$\begin{aligned} &\operatorname{Tr}_{L^2(\Lambda)}\left\{H_{\text{eff}}^{(g)}(\gamma_{\text{per}})\,(\gamma - \gamma_{\text{per}})\right\} \\ &= \operatorname{Tr}_{L^2(\Lambda)}\left\{|H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n|\,\gamma_{\text{per}}^\perp\,\gamma\,\gamma_{\text{per}}^\perp - |H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n|\,\gamma_{\text{per}}\,\gamma\,\gamma_{\text{per}}\right\} \\ &\qquad - \operatorname{Tr}_{L^2(\Lambda)}\left\{\left(H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n\right)\gamma_{\text{per}}\right\} \\ &= \operatorname{Tr}_{L^2(\Lambda)}\left\{|H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) - e_n|\left(\gamma_{\text{per}}^\perp\,\gamma\,\gamma_{\text{per}}^\perp - \gamma_{\text{per}}\,\gamma^\perp\,\gamma_{\text{per}}\right)\right\}. \end{aligned}$$

By assumption γ is a projection, thus

$$\begin{aligned} (\gamma - \gamma_{\text{per}})^2 &= \gamma^2 + \gamma_{\text{per}}^2 - \gamma\,\gamma_{\text{per}} - \gamma_{\text{per}}\,\gamma \\ &= \gamma + \gamma_{\text{per}} - \gamma\,\gamma_{\text{per}} - \gamma_{\text{per}}\,\gamma \\ &= \gamma_{\text{per}}\,\gamma^\perp + \gamma\,\gamma_{\text{per}}^\perp \end{aligned} \tag{2.38}$$

Since

$$\gamma_{\rm per}\,\gamma^{\perp}\,\gamma_{\rm per}^{\perp} = -\gamma_{\rm per}\,\gamma\,\gamma_{\rm per}^{\perp}.$$

Equation (2.38) can be written

$$\begin{aligned}(\gamma-\gamma_{\rm per}\,)^2 &= \gamma_{\rm per}\,\gamma^{\perp}\,\gamma_{\rm per} + \gamma_{\rm per}\,\gamma^{\perp}\,\gamma_{\rm per}^{\perp} + \gamma_{\rm per}^{\perp}\,\gamma\,\gamma_{\rm per}^{\perp} + \gamma_{\rm per}\,\gamma\,\gamma_{\rm per}^{\perp}\\ &= \gamma_{\rm per}\,\gamma^{\perp}\,\gamma_{\rm per} + \gamma_{\rm per}^{\perp}\,\gamma\,\gamma_{\rm per}^{\perp}.\end{aligned}$$

Thus,

$$\mathrm{Tr}_{L^2(\Lambda)}\{H_{\rm eff}^{(g)}(\gamma_{\rm per})(\gamma-\gamma_{\rm per})\} = \mathrm{Tr}_{L^2(\Lambda)}\{|H_{\rm eff}^{(g)}(\gamma_{\rm per})-e_n|\,(\gamma-\gamma_{\rm per})^2\}.$$

Furthermore, we can write

$$Q\,(\gamma-\gamma_{\rm per},\gamma-\gamma_{\rm per}) = D\left(\rho_{(\gamma-\gamma_{\rm per})},\rho_{(\gamma-\gamma_{\rm per})}\right) - P(\gamma-\gamma_{\rm per}),$$

where

$$\begin{aligned}D(f,g) &= \int_\Lambda\int_\Lambda f(x)\,g(y)\,W(x-y)\,dx\,dy\\ P(\eta,\gamma) &= \int_\Lambda\int_\Lambda \overline{\eta(x,y)}\,\gamma(x,y)\,W(x-y)\,dx\,dy.\end{aligned}$$

Since $\lambda\in[0,1]$ we prove that

$$\mathrm{Tr}_{L^2(\Lambda)}\{|H_{\rm eff}^{(g)}(\gamma_{\rm per})-e_n|\,(\gamma-\gamma_{\rm per})^2\} + \frac{g}{2}\left\{D\left(\rho_{(\gamma-\gamma_{\rm per})},\rho_{(\gamma-\gamma_{\rm per})}\right) - P(\gamma-\gamma_{\rm per})\right\}$$

is positive. We first notice that, for $W\ge 0$, the direct term

$$D\left(\rho_{(\gamma-\gamma_{\rm per})},\rho_{(\gamma-\gamma_{\rm per})}\right) = \int_\Lambda\int_\Lambda \rho_{(\gamma-\gamma_{\rm per})}(x)\,\rho_{(\gamma-\gamma_{\rm per})}(y)\,W(x-y)\,dx\,dy,$$

is positive. Therefore, it is enough to show that

$$P(\gamma-\gamma_{\rm per}) \le c\,\mathrm{Tr}_{L^2(\Lambda)}\left\{|H_{\rm eff}^{(g)}(\gamma_{\rm per})-e_n|\,(\gamma-\gamma_{\rm per})^2\right\}.$$

for a suitable constant c. We have

$$P(\gamma-\gamma_{\rm per}) = \int_\Lambda\int_\Lambda |\,(\gamma-\gamma_{\rm per})\,(x,y)|^2\,W(x-y)\,dx\,dy.$$

According to (2.35) we obtain

$$P(\gamma-\gamma_{\rm per}) \le c\int_\Lambda\int_\Lambda \frac{|\,(\gamma-\gamma_{\rm per})\,(x,y)|^2}{d_\Lambda(x-y)}\,dx\,dy.$$

Now Kato's inequality ([15], V, Formula(5.33), see also [31] or [12]) for all Schwarz functions $u \in S(\mathbb{R}^d)$, $d \geq 2$,

$$\int_{\mathbb{R}^d} \frac{|u(x)|^2}{|x|} dx \leq c_d^2 \int_{\mathbb{R}^d} |p| \, |\hat{u}(p)|^2 \, dp \leq c_d^2 \, \langle u| \, |\nabla| \, u \rangle$$

where

- c_d is the best possible constant for general values $d \geq 2$. It is defined for $1 < q < 2d$ and $q' = \frac{q}{q-1}$ by

$$c_d := \frac{\Gamma\left[\frac{1}{2}\left(\frac{d}{q} - \frac{1}{2}\right)\right] \Gamma\left[\frac{d}{2q'}\right]}{\sqrt{2}\, \Gamma\left[\frac{1}{2}\left(\frac{d}{q'} + \frac{1}{2}\right)\right] \Gamma\left[\frac{d}{2q}\right]},$$

  with Γ denotes the gamma function.

- and the Fourier transform of the function u is given by

$$\hat{u}(p) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-ipx} \, u(x) \, dx.$$

In particular

$$c_3 = \sqrt{\pi/2}, \quad c_2 = \frac{\Gamma[1/4]}{\sqrt{2}\,\Gamma[3/4]}.$$

gives for any fixed x, that

$$\langle k(x,.)| \, \frac{1}{|x - .|} \, k(x,.) \rangle_{L^2(\mathbb{R}^d)} \leq c_d^2 \, \langle k(x,.)||\nabla|k(x,.)\rangle_{L^2(\mathbb{R}^d)}. \tag{2.39}$$

To apply Kato's inequality in our case we remark

$$\int_\Lambda \int_\Lambda \frac{|(\gamma - \gamma_{\text{per}})\,(x,y)|^2}{d_\Lambda(x-y)} \, dx \, dy \leq \int_\Lambda \int_\Lambda \frac{|(\gamma - \gamma_{\text{per}})\,(x,y)|^2 \, \chi^2\left(\frac{d_\Lambda(x-y)}{R}\right)}{d_\Lambda(x-y)} \, dx \, dy,$$

where χ is a non-negative cut-off function on Λ and $R < \frac{L}{2}$. But the function $d_\Lambda(x-y)^{-1} \, \chi^2\left(\frac{d_\Lambda(x-y)}{R}\right)$ has a unique extension by 0 in $\mathbb{R}^d$, this yields

$$\int_\Lambda \int_\Lambda \frac{|(\gamma - \gamma_{\text{per}})\,(x,y)|^2}{d_\Lambda(x-y)} \, dx \, dy \leq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{|(\gamma - \gamma_{\text{per}})\,(x,y)|^2 \, \chi^2\left(\frac{|x-y|}{R}\right)}{|x-y|} \, dx \, dy.$$

Using now the fact that $\forall \varepsilon > 0 : \, |\nabla| \leq \frac{1}{2}\,\varepsilon\,(-\Delta) + \frac{1}{2\varepsilon} \cdot \mathbb{1}$, we obtain

$$\begin{aligned}\langle \chi u|\,|\nabla|\,\chi u\rangle &\leq \frac{1}{2\varepsilon}\,\|\chi u\|^2 + \frac{\varepsilon}{2}\,\|\nabla \chi u\|^2 \\ &= \frac{1}{2\varepsilon}\,\|\chi u\|^2 + \frac{\varepsilon}{2}\,\|(\nabla\chi)\,u + \chi\,(\nabla u)\|^2 \\ &\leq \left(\frac{1}{2\varepsilon} + \frac{\varepsilon}{2}\,\|\nabla\chi\|_\infty^2\right) \cdot \|u\|^2 + \varepsilon\,\|\nabla u\|^2\,,\end{aligned}$$

Therefore with (2.39) we get

$$\begin{aligned}&P(\gamma - \gamma_{\mathrm{per}}) \\ &\leq c_d^2 \left\langle \chi\Big(\frac{|x-\cdot|}{R}\Big)\,(\gamma-\gamma_{\mathrm{per}})\,(x,\cdot)\Big|\,|\nabla|\,\chi\Big(\frac{|x-.|}{R}\Big)\,(\gamma-\gamma_{\mathrm{per}})\,(x,\cdot)\right\rangle_{L^2(\mathbb{R}^d)} \\ &\leq c_d^2\,\varepsilon \left\langle (\gamma-\gamma_{\mathrm{per}})\,(x,\cdot)\Big|\,|\nabla|^2\,(\gamma-\gamma_{\mathrm{per}})\,(x,\cdot)\right\rangle + c_d^2 \left(\frac{1}{2\varepsilon} + \frac{\varepsilon}{2}\,\|\nabla\chi\|_\infty^2\right) \|(\gamma-\gamma_{\mathrm{per}})\,(x,\cdot)\|_{L^2(\Lambda)}^2 \\ &\leq c_d^2\,\varepsilon\,\mathrm{Tr}_{L^2(\Lambda)}\left\{\left(|\nabla|^2 \otimes \mathbb{1}\right)(\gamma-\gamma_{\mathrm{per}})^2\right\} + c_d^2 \left(\frac{1}{2\varepsilon} + \frac{\varepsilon}{2}\,\|\nabla\chi\|_\infty^2\right) \Big\|(\gamma-\gamma_{\mathrm{per}})\,(x,\cdot)\Big\|_{L^2(\Lambda)}^2.\end{aligned}$$

Our goal is reached by showing

$$\exists C = C(a, V) \in \mathbb{R} : |\nabla|^2 \leq C\,|H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}}) - e_n|,$$

which is equivalent to prove that

$$-\Delta \leq C\,|H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}}) - e_n|.$$

Since the square root as an operator is a monotone function it suffices to prove

$$(-\Delta)^2 \leq C^2 \left(H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}}) - e_n\right)^2,$$

which is equivalent to the requirement

$$\|-\Delta\psi\|_{L^2(\Lambda)} \leq C \left\|\left(H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}}) - e_n\right)\psi\right\|_{L^2(\Lambda)},$$

for all $\psi \in \rho(\Lambda) \subseteq \mathfrak{H}_\Lambda$. We have

$$\|-\Delta\psi\|_{\mathfrak{H}_\Lambda} \leq \left\|\left(H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}}) - e_n\right)\psi\right\|_{L^2(\Lambda)} + \|V\psi\|_{L^2(\Lambda)}\,,$$

since V is $-\Delta$-bounded with a relative bound smaller than 1, we get

$$\|-\Delta\psi\|_{L^2(\Lambda)} \leq \left\|(H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}}) - e_n)\psi\right\|_{L^2(\Lambda)} + \alpha\,\|-\Delta\psi\|_{L^2(\Lambda)} + \beta\,\|\psi\|_{L^2(\Lambda)}\,. \tag{2.40}$$

Rearranging turns (2.40) into

$$(1-\alpha)\left\|-\Delta\psi\right\|_{L^2(\Lambda)} \leq \left\|\left(H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}})-e_n\right)\psi\right\|_{L^2(\Lambda)} + \beta\left\|\psi\right\|_{L^2(\Lambda)}, \tag{2.41}$$

since the effective Hamiltonian according to Lemma 2.5 has a gap above the energy level number N and $\sigma\left(H_{\mathrm{eff}}^{(g)}\right) \cap [-a,a] = \emptyset$ for $a>0$, we get from the spectral theorem that

$$\left\|\mathbb{1}\psi\right\|_{L^2(\Lambda)} \leq \left\|\frac{\left(H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}})-e_n\right)}{a}\psi\right\|_{L^2(\Lambda)},$$

substituting in (2.40) gives

$$\begin{aligned}(1-\alpha)\left\|-\Delta\psi\right\|_{L^2(\Lambda)} &\leq \left\|\left(H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}})-e_n\right)\psi\right\|_{L^2(\Lambda)} + \beta\left\|\frac{\left(H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}})-e_n\right)}{a}\psi\right\|_{L^2(\Lambda)} \\ &\leq \left(1+\frac{\beta}{a}\right)\left\|\left(H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}})-e_n\right)\psi\right\|_{L^2(\Lambda)}.\end{aligned}$$

Thus,

$$\left\|-\Delta\psi\right\|_{L^2(\Lambda)} \leq \frac{a+\beta}{a(1-\alpha)}\left\|\left(H_{\mathrm{eff}}^{(g)}(\gamma_{\mathrm{per}})-e_n\right)\psi\right\|_{L^2(\Lambda)}. \tag{2.42}$$

Therefore, γ_{per} is a minimizer of the HF functional defined on all density matrices in $\mathscr{L}^1(\mathfrak{H}_\Lambda)$. Since the periodic HF energy is larger than the unrestricted HF energy we then conclude the equality between them. $\square$

Chapter 3

Bloch Wave Decomposition and its Application to the Periodic Hartree-Fock Theory

Contents

Summary

To study the periodic properties of minimizers of (1.17) and to compute the fibers of a considered operator as explicitly as possible, we use Bloch analysis which generalizes Fourier analysis. In 3.1 an overview will be given on how to get such a decomposition from the spectral resolution of the unbounded self-adjoint Laplace operator. In this way a decomposition of functions in $\mathfrak{H}_\Lambda$ into Bloch waves will be constructed in 3.1.1 by considering a given invariance (translation invariance). But to this decomposition there corresponds a so-called direct integral decomposition of operators on $\mathfrak{H}_\Lambda$. This integral decomposition will be applied to the periodic density matrices to obtain an explicit formula for their fibers and to formulate equivalent statements for their periodicity. These results which are formed in Lemma 3.1, 3.2 and 3.5, will play an important role in the following chapters.

3.1 Fourier Waves and Spectral Decomposition

The spectral resolution[1] of the unbounded self-adjoint operator $A = -\Delta$ on $\mathcal{H} := L^2(\mathbb{R}^d)$ using plane waves (also called Fourier waves) $e^{ix\xi}$ can be generalized for any periodic unbounded self-adjoint operator A by considering Bloch waves. Such Bloch waves are regarded as the counterpart of the plane waves. First of all, let us recall how to get this resolution of $-\Delta$ with the aid of the plan waves $e^{ix\xi}$. Because of the relation

$$-\Delta\, e^{ix\xi} = |\xi|^2\, e^{ix\xi}, \tag{3.1}$$

the plane waves $e^{ix\xi}$ for $\xi \in \mathbb{R}^d$ can be considered as generalized eigenfunctions of $-\Delta$ even though they do not have finite energy. Moreover, the inverse Fourier transform

$$\left(\mathcal{F}^{-1} f\right)(x) = \frac{1}{(2\pi)^{d/2}} \int\limits_{\mathbb{R}^d} e^{ix\xi} f(\xi)\, d\xi,$$

can be interpreted as the resolution of the identity operator on $\mathcal{H}$ in terms of these generalized eigenfunctions. In particular, this shows that $\left\{e^{ix\xi} \mid \xi \in \mathbb{R}^d\right\}$ is a generalized basis for $\mathcal{H}$ and the resolution of the operator itself can be given in terms of this basis by

$$(-\Delta\, f)(x) = \frac{1}{(2\pi)^{d/2}} \int\limits_{\mathbb{R}^d} |\xi|^2\, e^{ix\xi} f(\xi)\, d\xi,$$

for all $x \in \mathbb{R}^d$ and $\mathcal{F}^{-1} f \in H^2(\mathbb{R}^d)$, which implies that the operator $-\Delta$ goes over to the multiplication operator by the polynomial $|\xi|^2$ on the Fourier side. More precisely,

$$\mathcal{F}(-\Delta f)(\xi) = |\xi|^2 \left(\mathcal{F} f\right)(\xi).$$

3.1.1 Bloch Wave Decomposition of $\mathfrak{H}_\Lambda$

We now consider the Hilbert space $\mathfrak{H}_\Lambda = L^2\left\{(\mathbb{R})^d/(L\mathbb{Z})^d\right\}$ with L be an integer and aim to construct the Bloch wave decomposition for functions $\varphi \in \mathfrak{H}_\Lambda$, through which we generalize the plane waves. For this purpose we introduce

- the unit cell $Q := \Lambda/\Gamma = \mathbb{R}^d/(q\mathbb{Z})^d$ of Λ centered at 0,
- the lattice $\Gamma := (q\mathbb{Z})^d/(L\mathbb{Z})^d$,
- the first Brillouin zone $Q^* = (\Lambda/\Gamma)^*$ (or the unit cell of the dual lattice associated to Γ).

[1] for more details see [35]

Moreover, we denote again by τ_k the translation operator on $\mathfrak{H}_\Lambda$ defined by

$$\Big(\tau_k\varphi\Big)(x) := \varphi(x+k), \tag{3.2}$$

for all $k \in \Gamma$. We notice that (3.1) can be generalized by fixing $\xi \in \Gamma^*$ and finding $\lambda = \lambda(\xi) \in \mathbb{C}$ and $\varphi = \varphi(x,\xi) \in \mathfrak{H}_\Lambda$ (nonzero) such that

$$A\,\varphi = \lambda\,\varphi,\ \ \varphi \text{ is } \Gamma\text{-periodic},$$

where the eigenvectors φ are known as Bloch waves and the eigenvalues are called Bloch eigenvalues. The Γ-periodicity of $\varphi \in \mathfrak{H}_\Lambda$ can be defined as in 1.2.1, namely:

Definition 3.1. *A function $\varphi : \Lambda \longrightarrow \mathbb{C}$ is said to be Γ-periodic if*

$$\left(\tau_k\varphi\right)(x) = \varphi(x), \tag{3.3}$$

for all $x \in \Lambda$ and $k \in \Gamma$.

To know what the functions $\varphi(x,\xi)$ look like, we must first construct a decomposition of $\mathfrak{H}_\Lambda$ according to the translation invariance property (3.3). The idea of such a decomposition has been introduced by Floquet [9] in the one-dimensional case and by Bloch [3] in the general case. We shall explain this method following the formalism of Reed and Simon [24] or that of Conca, Planchard and Vanninathan [4]. Therefore, we must decompose $\varphi \in \mathfrak{H}_\Lambda$ in terms of Γ-periodic functions. To this end, we associate to $\varphi(x)$ a function $\varphi_\sharp(x,\xi)$ as follows.

$$\varphi_\sharp(x,\xi) = \frac{1}{\ell^{d/2}}\sum_{k\in\Gamma} e^{-i\xi(x+k)}\varphi(x+k). \tag{3.4}$$

On the one hand, the function $\varphi_\sharp(x,\xi)$ is Γ-periodic with respect to x. Indeed, for each $m \in \Gamma$ we have

$$\begin{aligned}\varphi_\sharp(x+m,\xi) &= \frac{1}{\ell^{d/2}}\sum_{k\in\Gamma} e^{-i\xi(x+k+m)}\varphi(x+k+m)\\ &= \frac{1}{\ell^{d/2}}\sum_{k'\in\Gamma} e^{-i\xi(x+k')}\varphi(x+k'),\end{aligned}$$

since Γ is a group. On the other hand, the right side of (3.4) is a Fourier series expansion with respect to $\xi \in \Gamma^*$ with coefficients in $\mathfrak{H}_Q := L^2\left(Q\right)$. Therefore, it follows that $\varphi_\sharp(x,\xi)$ is Q^*-periodic with respect to $\xi \in \Gamma^*$. Thus, we can write

$$\varphi(x) = \sum_{\xi\in\Gamma^*}\varphi_\sharp(x,\xi).$$

Thus,

$$\sum_{\xi\in\Gamma^*} |\varphi_\sharp(x,\xi)|^2 = \sum_{k\in\Gamma} |\varphi(x+k)|^2 .$$

Integrating the above equality with respect to $x \in Q$, we obtain

$$\begin{aligned}\int_Q \sum_{\xi\in\Gamma^*} |\varphi_\sharp(x,\xi)|^2\,dx &= \int_Q \sum_{k\in\Gamma} |\varphi(x+k)|^2\,dx \\ &= \int_\Lambda |\varphi(x)|^2\,dx. \end{aligned} \tag{3.5}$$

Hence, a unitary transformation is obtained, which is called the Floquet operator, given by

$$\begin{aligned} U : \mathfrak{H}_\Lambda &\longrightarrow \widetilde{\mathfrak{H}}_\Lambda := L^2\left(\Gamma^*; \mathfrak{H}_Q\right) \\ (U\varphi)_\xi\,(x) &:= \varphi_\sharp(x,\xi) = \frac{1}{\ell^{d/2}} \sum_{k\in\Gamma} e^{-i(x+k)\xi}\,\varphi(x+k), \end{aligned} \tag{3.6}$$

for $\xi \in \Gamma^*$, $x \in Q$ and $\varphi \in \mathfrak{H}_\Lambda$. Its inverse can be written explicitly and is given for all $\psi \in \widetilde{\mathfrak{H}}_\Lambda$ by the formula

$$\left(U^{-1}\psi\right)(x+k) = \ell^{-d/2} \sum_{\xi\in\Gamma^*} e^{i(x+k)\xi}\,\psi(x,\xi), \tag{3.7}$$

for all $k \in \Gamma$, $x \in Q$. The fact that U is unitary can be formulated as follows. For all $\varphi, \psi \in \mathfrak{H}_\Lambda$ using (3.6) and (3.7) we get

$$\sum_{\xi\in\Gamma^*} \left\langle (U\varphi)_\xi \mid (U\psi)_\xi \right\rangle_{\mathfrak{H}_Q} = \langle \varphi \mid \psi \rangle_{\mathfrak{H}_\Lambda}, \tag{3.8}$$

which can be proved again using Poisson's formula as follows:

$$\begin{aligned} \sum_{\xi\in\Gamma^*} \left\langle (U\varphi)_\xi \mid (U\psi)_\xi \right\rangle_{\mathfrak{H}_Q} &= \sum_{\xi\in\Gamma^*} \int_Q \overline{(U\varphi)_\xi\,(x)}\,(U\psi)_\xi\,(x)\,dx \\ &= \sum_{\xi\in\Gamma^*} \int_Q \ell^{-d} \sum_{k,l\in\Gamma} e^{ix(k-l)}\,\overline{\varphi(x+k)}\,\psi(x+l)\,dx. \end{aligned}$$

With Poisson's formula we obtain

$$\begin{aligned} \sum_{\xi\in\Gamma^*} \left\langle (U\varphi)_\xi \mid (U\psi)_\xi \right\rangle_{\mathfrak{H}_Q} &= \int_Q \sum_{k,l\in\Gamma} \delta_{k,l}\,\overline{\varphi(x+k)}\,\psi(x+l)\,dx \\ &= \int_Q \sum_{k\in\Gamma} \overline{\varphi(x+k)}\,\psi(x+k)\,dx \\ &= \int_\Lambda \overline{\varphi(x)}\,\psi(x)\,dx. \end{aligned}$$

In particular we get as in (3.5) that U is an isometry

$$\sum_{\xi\in\Gamma^*} \left\|(U\varphi)_\xi\right\|_{\mathfrak{H}_Q} = \|\varphi\|_{\mathfrak{H}_\Lambda} . \tag{3.9}$$

Remark 3.1. 1. It is convenient to consider $(U\varphi)_\xi$ as a function lying in $\mathfrak{H}_Q^\xi$ with

$$\mathfrak{H}_Q^\xi := \left\{\varphi \in \mathfrak{H}_Q \middle| \, e^{-ix\xi}\,\varphi(x) \text{ is } \Gamma\text{-periodic } \right\},$$

which is isomorphic to $\mathfrak{H}_Q$ with respect to the usual Hilbert scalar product on $\mathfrak{H}_Q$.

2. If φ is Γ-periodic, then

$$(U\varphi)_\xi\,(x) = \delta_{\xi,0}\,\ell^{d/2}\,e^{-i\xi x}\,\varphi(x) = \delta_{\xi,0}\,e^{-i\xi x}\,\ (U\varphi)_0\,(x).$$

For the first equality one has

$$(U\varphi)_\xi\,(x) = \frac{1}{\ell^{d/2}}\sum_{k\in\Gamma} e^{-i\xi(x+k)}\,\varphi(x+k) = \frac{1}{\ell^{d/2}}\,\varphi(x)\sum_{k\in\Gamma} e^{-i\xi(x+k)}.$$

Poisson's formula gives

$$(U\varphi)_\xi\,(x) = \ell^{d/2}\,\delta_{\xi,0}\,e^{-i\xi x}\,\varphi(x).$$

The second equality follows from the fact that $(U\varphi)_0\,(x) = \ell^{d/2}\varphi(x)$.

3.2 Bloch Wave Decomposition of the Density Matrix γ

We can now use the isometry U to construct the spectral decomposition of a Γ-periodic, self-adjoint operator γ on $\mathfrak{H}_\Lambda$ which is the periodic density matrix we are looking for, where the Γ-periodicity of γ reads as follows

$$\forall k \in \Gamma : \tau_k\gamma = \gamma\tau_k. \tag{3.10}$$

The decomposition of functions in $\mathfrak{H}_\Lambda$ into Bloch waves corresponds to a direct integral decomposition of γ in the sense that there is a unique bounded operator-valued function $\xi \longmapsto \gamma_\xi$, such that for every $\varphi \in \mathfrak{H}_\Lambda$ and $\xi \in \Gamma^*$ we have

$$(U\gamma\varphi)_\xi := \gamma_\xi\,(U\varphi)_\xi\,. \tag{3.11}$$

Moreover, we have

$$\|\gamma\|_{\mathscr{B}(\mathfrak{H}_\Lambda)} = \sup\Big\{\|\gamma_\xi\|_{\mathscr{B}\left(\mathfrak{H}_Q\right)} \,\Big|\, \xi \in \Gamma^*\Big\}.$$

We shall write

$$\gamma = |\Gamma|^{-1} \bigoplus_{\xi\in\Gamma^*} \gamma_\xi$$

in order to refer to the decomposition (3.11) of γ. This means we have reduced the spectral analysis of γ into its family of self-adjoint operators $\gamma_\xi \in \mathscr{B}\left(\mathfrak{H}_Q^\xi\right)$. We will now study the properties of this family when γ is an arbitrary self-adjoint operator satisfying

1. γ commutes with the translations which leave the periodic lattice Γ invariant, i.e., γ satisfies (3.10).
2. the 1-pdm γ fulfills $0 \leq \gamma \leq \mathbb{1}$, where $\mathbb{1}$ is the identity operator on $\mathfrak{H}_\Lambda$.

The following lemma gives an equivalent formulation of (3.10) in terms of its kernel $\gamma(.,.)$.

Lemma 3.1. *Let $\gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda)$ be a self-adjoint operator. Then γ is Γ-periodic in the sense of* (3.10) *if and only if*

$$\forall k \in \Gamma : \gamma(x+k, y+k) = \gamma(x,y).$$

Proof. Since γ is a compact self-adjoint operator, it is diagonalizable. Thus, there always exists $\{\lambda_n\}_{n=1}^\infty \subseteq \mathbb{R}_0^+$ with $\sum\limits_{n=1}^\infty \lambda_n = \mathrm{Tr}_{\mathfrak{H}_\Lambda}(\gamma)$ and an orthonormal basis $\{\varphi_n\}_{n=1}^\infty \subseteq \mathfrak{H}_\Lambda$ such that

$$\gamma = \sum_{n=1}^\infty \lambda_n |\varphi_n\rangle\langle\varphi_n|.$$

Therefore its kernel is well-defined and for $x, y \in \Lambda$ is given by

$$\gamma(x,y) = \sum_{n=1}^\infty \lambda_n \,\overline{\varphi_n(x)}\,\varphi_n(y).$$

Now we assume that

$$(\gamma\varphi)(x) = \int\limits_\Lambda \gamma(x,y)\,\varphi(y)dy, \tag{3.12}$$

for any function $\varphi \in \mathfrak{H}_\Lambda$. Then

$$\begin{aligned}(\tau_k\gamma\varphi)(x) &= (\gamma\varphi)(x+k)\\ &= \int\limits_\Lambda \gamma(x+k,y)\varphi(y)dy. \end{aligned}\tag{3.13}$$

By setting $y = y + k \in \Lambda$, we deduce

$$(\tau_k \, \gamma \, \varphi) \, (x) = \int\limits_\Lambda \gamma(x+k, y+k) \, \varphi(y+k) \, dy. \tag{3.14}$$

Moreover,

$$\begin{aligned}(\gamma \, \tau_k \, \varphi_k) \, (x) &= \int\limits_\Lambda \gamma(x, y) \, \Big(\tau_k \varphi \Big)(y) \, dy \\ &= \int\limits_\Lambda \gamma(x, y) \, \varphi(y+k) \, dy\end{aligned}$$

But according to the hypothesis of the lemma we have for all $\varphi \in \mathfrak{H}_\Lambda$ and $k \in \Gamma$ that

$$(\tau_k \, \gamma \, \varphi) \, (x) = (\gamma \, \tau_k \, \varphi) \, (x),$$

which implies owing to (3.13) and (3.14) that

$$\gamma(x+k, y+k) = \gamma(x, y).$$

$\square$

In addition, any periodic operator is unitarily equivalent to a direct sum of operators on $\mathfrak{H}_Q$.

Lemma 3.2. *For all $\gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda)$, if γ is Γ-periodic, we have for all $\psi \in \mathfrak{H}_\Lambda$*

$$(U\gamma\psi)_\xi = \gamma_\xi (U\psi)_\xi, \quad \forall \xi \in \Gamma^*$$

where $\gamma_\xi \in \mathscr{L}^1(\mathfrak{H}_Q)$ is given by

$$\begin{aligned}\gamma_\xi(x, y) &= e^{-i\xi(x-y)} \sum_{k \in \Gamma} e^{-i\xi k} \gamma(x+k, y) \\ &= e^{-i\xi(x-y)} \sum_{k \in \Gamma} e^{i\xi k} \gamma(x, y+k)\end{aligned} \tag{3.15}$$

Moreover,

$$\gamma = U^{-1} \Big(\bigoplus_{\xi \in \Gamma^*} \gamma_\xi \Big) U \, .$$

The proof is an adaptation to a bounded domain and finite dimensions of the proof in [14].

Proof. It follows from the definition (3.6) of U that $\forall \xi \in \Gamma^*$ and $\forall x \in Q$:

$$\begin{aligned}
(U\gamma\psi)_\xi (x) &= \frac{1}{|\Gamma|^{\frac{1}{2}}} \sum_{k\in\Gamma} e^{-i\xi(x+k)} (\gamma\psi)(x+k) \\
&= \frac{1}{|\Gamma|^{\frac{1}{2}}} \sum_{k\in\Gamma} e^{-i\xi(x+k)} \int\limits_{\Lambda} \gamma(x+k,y)\psi(y)dy \\
&= \frac{1}{|\Gamma|^{\frac{1}{2}}} \sum_{k\in\Gamma} e^{-i\xi(x+k)} \left\langle \overline{\gamma(x+k,.)} | \psi \right\rangle_{\mathfrak{H}_\Lambda}.
\end{aligned}$$

Using the unitarity of U, this implies

$$\begin{aligned}
(U\gamma\psi)_\xi (x) &= \frac{1}{|\Gamma|^{\frac{1}{2}}} \sum_{k\in\Gamma} e^{-i\xi(x+k)} \sum_{\xi'\in\Gamma^*} \langle \left(U\overline{\gamma(x+k,.)} \right)_{\xi'} | (U\psi)_{\xi'} \rangle_{\mathfrak{H}_Q} \\
&= \frac{1}{|\Gamma|^{\frac{1}{2}}} \sum_{k\in\Gamma} e^{-i\xi(x+k)} \sum_{\xi'\in\Gamma^*} \int\limits_{Q} \overline{\left(U\overline{\gamma(x+k,.)} \right)_{\xi'} (y)} (U\psi)_{\xi'}(y)dy \\
&= \frac{1}{|\Gamma|} \sum_{k\in\Gamma} e^{-i\xi(x+k)} \sum_{\xi'\in\Gamma^*} \int_Q \overline{\sum_{k'\in\Gamma} e^{-i\xi'(y+k')} \overline{\gamma(x+k,y+k')}} (U\psi)_{\xi'}(y)dy \\
&= \frac{1}{|\Gamma|} \sum_{\xi'\in\Gamma^*} \int_Q \sum_{k,k'\in\Gamma} e^{-i\xi(x+k)} e^{i\xi'(y+k')} \gamma(x+k,y+k')(U\psi)_{\xi'}(y)dy.
\end{aligned}$$

Since the density matrix γ is Γ-periodic, we get

$$\begin{aligned}
(U\gamma\psi)_\xi (x) &= \frac{1}{|\Gamma|} \sum_{\xi'\in\Gamma^*} \int_Q \sum_{k,k'\in\Gamma} e^{-i\xi(x+k)} e^{i\xi'(y+k')} \gamma(x+k-k',y)(U\psi)_{\xi'}(y)dy \\
&= \frac{1}{|\Gamma|} \sum_{\xi'\in\Gamma^*} \int_Q \sum_{k,k'\in\Gamma} e^{-i\xi(x+k+k')} e^{i\xi'(y+k')} \gamma(x+k,y)(U\psi)_{\xi'}(y)dy \\
&= \frac{1}{|\Gamma|} \sum_{\xi'\in\Gamma^*} \int_Q \sum_{k\in\Gamma} \left(\sum_{k'\in\Gamma} e^{i(\xi'-\xi)k'} \right) e^{-i\xi(x+k)} e^{i\xi' y} \gamma(x+k,y)(U\psi)_{\xi'}(y)dy.
\end{aligned}$$

With the Poisson summation formula

$$\sum_{k\in\Gamma} e^{i\xi k} = |\Gamma| \, \delta_{\xi,0}, \quad \forall \xi \in \Gamma^*,$$

we have

$$\begin{aligned}
(U\gamma\psi)_\xi (x) &= \sum_{\xi'\in\Gamma^*} \int_Q \sum_{k\in\Gamma} \delta_{\xi,\xi'} e^{-i\xi(x+k)} e^{i\xi' y} \gamma(x+k,y)(U\psi)_{\xi'}(y)dy \\
&= \int_Q \big(e^{-i\xi(x-y)} \sum_{k\in\Gamma} e^{-i\xi k} \gamma(x+k,y) \big) (U\psi)_\xi(y)dy \\
&= \gamma_\xi \, (U\psi)_\xi(x), \qquad (3.16)
\end{aligned}$$

where $\gamma_\xi \in \mathscr{L}(\mathfrak{H}_Q)$ is the operator with kernel $\gamma_\xi(x,y)$ defined in (3.15).

□

The above lemma allows us to give another property of the fibers of γ.

Lemma 3.3. *Let γ be a self-adjoint operator on $\mathfrak{H}_\Lambda$. Then γ is Γ-periodic if and only if*

$$\left(U\,\gamma\,U^{-1}\right)(x,\xi;y,\eta) = \gamma\,(x,\xi;y,\xi)\;\delta_{\xi,\eta}.$$

Proof. We assume as in (3.12) that $\gamma(x,y)$ is a kernel of γ. Then for any $\varphi \in \mathfrak{H}_\Lambda$ we can write

$$\left(U\,\gamma\,U^{-1}\,\varphi\right)(x,\xi) = \int_Q \left(U\,\gamma\,U^{-1}\right)(x,\xi;y,\eta)\,\varphi\,(y,\eta)\,dy.$$

On the other hand (3.16) and (3.15) yield

$$\begin{aligned}\left(U\,\gamma\,U^{-1}\,\varphi\right)(x,\xi) &= \int_Q e^{-i\xi(x-y)} \sum_{\ell\in\Gamma} e^{-i\xi\ell}\,\gamma\,(x+\ell;y)\;\varphi(y,\xi)\,dy \\ &= \int_Q \gamma\,(x,\xi;y,\xi)\,\delta_{\eta,\xi}\varphi(y,\eta)dy,\end{aligned}$$

hence the claim. □

Bloch's theorem states that the eigenvectors of a Hamiltonian with periodic potential can be chosen so that any eigenvector belongs to $\mathfrak{H}_\Lambda^\xi$ for a given $\xi \in \Gamma^*$, where

$$\mathfrak{H}_\Lambda^\xi := \left\{ u \in \mathfrak{H}_\Lambda \middle|\, e^{-i\xi x}\,u \;\text{ is }\; \Gamma\text{-periodic}\right\}.$$

In the following two lemmas a Bloch theorem for any self-adjoint Γ-periodic operator on $\mathfrak{H}_\Lambda$ is given.

Lemma 3.4. *For any sequence $(\gamma_\xi)_{\xi\in\Gamma^*}$ such that $\forall\xi \in \Gamma^*$, $\gamma_\xi \in \mathscr{L}^1(\mathfrak{H}_Q)$ satisfies*

$$\gamma_\xi = \sum_{j\in\mathbb{N}} \lambda_{\xi,j}\;|\varphi_{\xi,j}\rangle\langle\varphi_{\xi,j}| \tag{3.17}$$

where $\lambda_{\xi,j} \in \mathbb{C}$ and $\varphi_{\xi,j} \in \mathfrak{H}_Q$, the operator $\gamma = U^{-1}\left(\bigoplus_{\xi\in\Gamma^*}\gamma_\xi\right)U \,\in\, \mathscr{L}(\mathfrak{H}_\Lambda)$ satisfies:

$$\gamma = \sum_{\xi\in\Gamma^*}\,\sum_{j\geq 1} \lambda_{\xi,j}\,|\psi_{\xi,j}\rangle\langle\psi_{\xi,j}|\,,$$

where $\psi_{\xi,j} = \frac{1}{|\Gamma|^{\frac{1}{2}}}\,e^{i\xi x}\,\varphi_{\xi,j} \;\in\; \mathfrak{H}_\Lambda^\xi$.

Proof. If $\delta_{\xi_0,\xi}$ denotes the operator acting on $\mathscr{L}^1(\mathfrak{H}_Q)$ by multiplication with the Kronecker symbol $\delta_{\xi_0,\xi}$, the following decomposition of the identity holds

$$\mathbb{1}_{\widetilde{\mathfrak{H}}_\Lambda} = \sum_{\xi_0 \in \Gamma^*} \bigoplus_{\xi \in \Gamma^*} \delta_{\xi_0,\xi}$$

Therefore, it holds that

$$\gamma = U^{-1} \left(\sum_{\xi_0 \in \Gamma^*} \bigoplus_{\xi \in \Gamma^*} \delta_{\xi_0,\xi} \right) \left(\bigoplus_{\xi \in \Gamma^*} \gamma_\xi \right) U = \sum_{\xi_0 \in \Gamma^*} U^{-1} \left[\bigoplus_{\xi \in \Gamma^*} \left(\delta_{\xi_0,\xi} \gamma_\xi \right) \right] U. \tag{3.18}$$

Moreover, using (3.17) and the unitarity of U we get for all $\varphi \in \mathfrak{H}_Q$ and $\xi \in \Gamma^*$:

$$\begin{aligned}
\left(\bigoplus_{\xi' \in \Gamma^*} \left(\delta_{\xi_0,\xi'} \gamma_{\xi'} \right) U \varphi \right)_\xi &= \delta_{\xi_0,\xi}\, \gamma_\xi\, (U\varphi)_\xi \\
&= \delta_{\xi_0,\xi} \sum_{j \in \mathbb{N}} \lambda_{\xi,j}\, \varphi_{\xi,j}\, \langle \varphi_{\xi,j} |\, (U\varphi)_\xi \rangle_{\mathfrak{H}_Q} \\
&= \sum_{j \in \mathbb{N}} \lambda_{\xi_0,j}\, \left(\delta_{\xi_0,\xi}\, \varphi_{\xi_0,j} \right) \langle \varphi_{\xi_0,j} |\, (U\varphi)_{\xi_0} \rangle_{\mathfrak{H}_Q} \\
&= \sum_{j \in \mathbb{N}} \lambda_{\xi_0,j}\, \left(\delta_{\xi_0,\xi}\, \varphi_{\xi_0,j} \right) \sum_{\xi' \in \Gamma^*} \langle \delta_{\xi_0,\xi'} \varphi_{\xi_0,j} |\, (U\varphi)_{\xi'} \rangle_{\mathfrak{H}_Q} \\
&= \sum_{j \in \mathbb{N}} \lambda_{\xi_0,j}\, \left(\delta_{\xi_0,\cdot}\, \varphi_{\xi_0,j} \right)_\xi \sum_{\xi' \in \Gamma^*} \langle \left(\delta_{\xi_0,\cdot} \varphi_{\xi_0,j} \right)_{\xi'} |\, (U\varphi)_{\xi'} \rangle_{\mathfrak{H}_Q} \\
&= \sum_{j \in \mathbb{N}} \lambda_{\xi_0,j}\, \left(\delta_{\xi_0,\cdot}\, \varphi_{\xi_0,j} \right)_\xi \langle U^{-1} \left(\delta_{\xi_0,\cdot} \varphi_{\xi_0,j} \right) | \varphi \rangle_{\mathfrak{H}_\Lambda},
\end{aligned}$$

which, in other words is

$$\bigoplus_{\xi \in \Gamma^*} \left(\delta_{\xi_0,\xi}\, \gamma_\xi \right) U = \sum_{j \geq 1} \lambda_{\xi_0,j}\, |\delta_{\xi_0,\cdot}\, \varphi_{\xi_0,j} \rangle \langle U^{-1} \left(\delta_{\xi_0,\cdot} \varphi_{\xi_0,j} \right) |, \tag{3.19}$$

where $\delta_{\xi_0,\cdot}\, \varphi_{\xi_0,j} \in \widetilde{\mathfrak{H}}_\Lambda$ denotes the function with fiber elements $\left(\delta_{\xi_0,\cdot} \varphi_{\xi_0,j} \right)_\xi = \delta_{\xi_0,\xi} \varphi_{\xi_0,j}$ for all $\xi \in \Gamma^*$. Set $\psi_{\xi_0,j} = U^{-1} \left(\delta_{\xi_0,\cdot} \varphi_{\xi_0,j} \right) \in \mathfrak{H}_\Lambda$. Then, putting equations (3.18) and (3.19) together, we get

$$\gamma = \sum_{\xi_0 \in \Gamma^*} \sum_{j \in \mathbb{N}} \lambda_{\xi_0,j}\, |\psi_{\xi_0,j} \rangle \langle \psi_{\xi_0,j} |\,.$$

Also, the explicit formula (3.7) for U^{-1} gives

$$\psi_{\xi_0,j} = \frac{1}{|\Gamma|^{\frac{1}{2}}}\, e^{i\xi_0 x}\, \varphi_{\xi_0,j},$$

where $\varphi_{\xi_0,j} \in \mathfrak{H}_Q$ and $\psi_{\xi_0,j}$, considered as an element of $\mathfrak{H}_\Lambda$, is Γ-periodic.

$\square$

Lemma 3.5 (Bloch's theorem). *Let $\gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda)$ be a Γ-periodic, self-adjoint operator. Then there exists a set $(\lambda_j)_{j\in\mathbb{N}}$ in $\mathbb{R}$ and an orthonormal sequence of vectors $(\psi_j)_{j\in\mathbb{N}}$ in $\mathfrak{H}_\Lambda$ such that*

$$\forall\, j \in \mathbb{N}\,,\ \exists \xi \in \Gamma^* \ \ s.t.\ \ \psi_j \in \mathfrak{H}_\Lambda^\xi, \tag{3.20}$$

and

$$\gamma = \sum_{j\in\mathbb{N}} \lambda_j \,|\psi_j\rangle\langle\psi_j|\ . \tag{3.21}$$

Proof. Since $\gamma = \gamma^*$, it follows that $\forall \xi \in \Gamma^*$, the operator γ_ξ given in Lemma 3.2 satisfies $(\gamma_\xi)^* = \gamma_\xi$. Therefore, there exists a set $(\lambda_{\xi,j})_{j\in\mathbb{N}}$ in $\mathbb{R}$ and an orthonormal set of vectors $(\varphi_{\xi,j})_{j\in\mathbb{N}}$ in $\mathfrak{H}_Q$ such that

$$\gamma_\xi = \sum_{j\in\mathbb{N}} \lambda_{\xi,j} \,|\varphi_{\xi,j}\rangle\langle\varphi_{\xi,j}|\ .$$

Using Lemma 3.4, we get

$$\gamma = \sum_{\xi\in\Gamma^*} \sum_{j\geq 1} \lambda_{\xi,j} \,|\psi_{\xi,j}\rangle\langle\psi_{\xi,j}|\ , \tag{3.22}$$

where

$$\psi_{\xi,j} = \frac{1}{|\Gamma|^{\frac{1}{2}}}\, e^{i\xi x}\, \varphi_{\xi,j} \ \in\ \mathfrak{H}_\Lambda^\xi\,. \tag{3.23}$$

By changing the name of the variables, equation (3.22) gives (3.21). The property $\lambda_j \in \mathbb{R}$ is then a consequence of $\lambda_{\xi,j} \in \mathbb{R}$ and (3.20) is a consequence of (3.23). It remains to show the orthonormality of $\psi_{\xi,j}$ to complete the proof. It follows from (3.23) for all $\xi_0 \in \Gamma^*$ that

$$\Big(U\psi_{\xi_0,j}\Big)_\xi = \delta_{\xi_0,\xi}\, \varphi_{\xi_0,j}.$$

Therefore, $\forall\, \xi_0, \xi_0' \in \Gamma^*$ and $\forall\, j, j' \geq 1$ we have

$$\begin{aligned}
\langle\psi_{\xi_0,j}|\psi_{\xi_0',j'}\rangle_{\mathfrak{H}_\Lambda} &= \sum_{\xi\in\Gamma^*} \langle (U\psi_{\xi_0,j})_\xi \,|\, \Big(U\psi_{\xi_0',j'}\Big)_\xi\rangle_{\mathfrak{H}_Q} \\
&= \sum_{\xi\in\Gamma^*} \delta_{\xi_0,\xi}\, \delta_{\xi_0',\xi}\, \langle \varphi_{\xi_0,j}, \varphi_{\xi_0',j'}\rangle_{\mathfrak{H}_Q} \\
&= \delta_{\xi_0,\xi_0'}\, \delta_{j,j'}.
\end{aligned}$$

□

Chapter 4

Characterization of periodic minimizers

Contents

Summary

In this chapter the fibers of the effective Hamiltonian will be given explicitly using Lemma 3.2. We should take advantage of that to compute also the fibers of the HF functional. These results will be set together to generalize Lieb's variational principle in the periodic case. Finally we make use of the proof of Lieb's variational principle to obtain a gap estimate on the fiber effective Hamiltonian.

4.1 Linearization, the Fibers of the Effective Hamiltonian

Let $\Lambda = \mathbb{R}^d/(L\mathbb{Z})^d$ be a torus with L be an integer. The length L is assumed to be of the form $L = \ell \cdot q$ where $\ell, q \in \mathbb{N}$. To study the periodic properties of minimizers of the HF functional with period Γ, we introduce the lattice $\Gamma = (q\mathbb{Z})^d/(L\mathbb{Z})^d$ and the unite cell $Q = \Lambda/\Gamma = \mathbb{R}^d/(q\mathbb{Z})^d$. The one-particle free Hamiltonian we will consider is

$$h = -\Delta + V,$$

where $-\Delta$ is the Laplace operator acting on $\mathfrak{H}_\Lambda = L^2(\Lambda)$ and the external potential V satisfies

$$V(x+k) = V(x), \quad \forall k \in \Gamma\,.$$

Let W be a positive function: $W(x) > 0$, $\forall x \in \Lambda$ such that

$$W(x) = W(-x), \quad \forall x \in \Lambda\,.$$

We will identify the pair-interaction potential W acting on $\mathfrak{H}_\Lambda \otimes \mathfrak{H}_\Lambda$ with the multiplication operator by $W(x-y)$. We are interested in the characterization of periodic minimizers of the HF functional defined for all $\gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda)$ by

$$\mathcal{E}_{\mathrm{hf}}(\gamma) = \mathrm{Tr}\{h\,\gamma\} + \frac{g}{2}\,Q(\gamma,\gamma), \tag{4.1}$$

where

$$Q(\gamma,\gamma') = \mathrm{Tr}\Big\{W(1-\mathrm{Ex})\Big(\gamma\otimes\gamma\Big)'\Big\}.$$

here

$$\mathrm{Ex} : f\otimes g \longmapsto g\otimes f$$

is the exchange operator on $\mathfrak{H}_\Lambda \otimes \mathfrak{H}_\Lambda$. The HF functional can be expanded as follows

$$\mathcal{E}_{\mathrm{hf}}(\gamma+\gamma') - \mathcal{E}_{\mathrm{hf}}(\gamma) = \mathrm{Tr}\{h\,\gamma'\} + g\,Q(\gamma,\gamma') + \frac{g}{2}\,Q(\gamma',\gamma')\,. \tag{4.2}$$

A direct computation shows that

$$Q(\gamma,\gamma') = \mathrm{Tr}\{W^1_\gamma\,\gamma'\} - \mathrm{Tr}\{W^2_\gamma\,\gamma'\},$$

where W^1_γ is the multiplication operator by the function

$$W^1_\gamma(x) = \int_\Lambda W(x-y)\,\gamma(y,y)dy, \tag{4.3}$$

and W^2_γ is the operator with kernel

$$W^2_\gamma(x,y) = W(x-y)\,\gamma(x,y)\,.$$

Then (4.2) rewrites as

$$\mathcal{E}_{\mathrm{hf}}(\gamma+\gamma') - \mathcal{E}_{\mathrm{hf}}(\gamma) = \mathrm{Tr}\{H^{(g)}_{\mathrm{eff}}\,\gamma'\} + \frac{g}{2}\,Q(\gamma',\gamma'), \tag{4.4}$$

where the effective Hamiltonian $H_{\text{eff}}^{(g)} \equiv H_{\text{eff}}^{(g)}(\gamma)$ is given by

$$H_{\text{eff}}^{(g)} = h + g\left(W_\gamma^1 - W_\gamma^2\right). \tag{4.5}$$

We remark that if γ is self-adjoint, then $H_{\text{eff}}^{(g)}$ is self-adjoint. Moreover, in the following lemma, we state that if γ is Γ-periodic, then $H_{\text{eff}}^{(g)}$ is Γ-periodic, and give the fibers of the effective Hamiltonian which will be used to obtain a fiber gap estimate.

Lemma 4.1. *For any Γ-periodic, self-adjoint operator $\gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda)$, the effective Hamiltonian $H_{\text{eff}}^{(g)}$ defined in (4.5) is Γ-periodic, self-adjoint operator on $\mathfrak{H}_\Lambda$ and its fiber is given by*

$$\forall \xi \in \Gamma^* : H_\xi^{(g)} = h_\xi + g\left(W_\gamma^1 - \left(W_\gamma^2\right)_\xi\right), \tag{4.6}$$

where W_γ^1 denotes the multiplication operator by the function $W_\gamma^1(x)$, $x \in Q$ defined in (4.3) and $\left(W_\gamma^2\right)_\xi$ is the operator with kernel

$$\left(W_\gamma^2\right)_\xi (x,y) = |\Gamma|^{-1/2} \sum_{\eta \in \Gamma^*} (UW)_{\xi-\eta}(x-y)\gamma_\eta(x,y),$$

for all $x, y \in Q$.

Proof. First the periodicity of $H_{\text{eff}}^{(g)}$ will be shown, i.e., $\tau_k\, H_{\text{eff}}^{(g)} = H_{\text{eff}}^{(g)}\, \tau_k$ for each $k \in \Gamma$, where τ_k denotes the translation operator defined in (3.2). For any $\varphi \in \mathfrak{H}_\Lambda$ we have

$$\left(\tau_k\, H_{\text{eff}}^{(g)}\, \varphi\right)(x) = (\tau_k\, h\, \varphi)(x) + g\left[\left(\tau_k\, W_\gamma^1\, \varphi\right)(x) - \left(\tau_k\, W_\gamma^2\, \varphi\right)(x)\right],$$

where for $h = -\Delta + V$ we have

$$[\tau_k\,(-\Delta + V)\,\varphi](x) = (-\Delta\,\varphi)(x+k) + (V\,\varphi)(x+k).$$

Since V is Γ-periodic and owing to the fact that there will not be any difference if we translate first and then make a derivation or vice versa we get

$$[\tau_k\,(-\Delta + V)\,\varphi](x) = (h\,\tau_k\,\varphi)(x).$$

The multiplication operator W_γ^1 commutes with τ_k, since

$$\begin{aligned}
\left(\tau_k\, W_\gamma^1\, \varphi\right)(x) &= \left(W_\gamma^1\, \varphi\right)(x+k) \\
&= W_\gamma^1(x+k)\,\varphi(x+k) \\
&= \left(\int_\Lambda \gamma(y,y)\, W(x+k-y)dy\right)\varphi(x+k).
\end{aligned}$$

By changing y to $y + k \in \Lambda$ we get

$$\left(\tau_k\, W^1_\gamma\, \varphi\right)(x) = \left(\int_\Lambda \gamma(y+k, y+k)\, W(x-y)\, dy\right) \varphi(x+k).$$

Since γ is Γ-periodic, then Lemma 3.1 implies that $\tau_k\, W^1_\gamma = W^1_\gamma\, \tau_k$. Similarly we prove the periodicity of the operator W^2_γ. Indeed, we have

$$\begin{aligned}\left(\tau_k\, W^2_\gamma\, \varphi\right)(x) &= \left(W^2_\gamma\, \varphi\right)(x+k) \\ &= \int_\Lambda \gamma(x+k, y)\varphi(y) W(x+k-y) dy.\end{aligned}$$

By changing y to $y + k$ and using the periodicity of γ we obtain

$$\begin{aligned}\left(\tau_k W^2_\gamma \varphi\right)(x) &= \int_\Lambda \gamma(x, y)\, \varphi(y+k)\, W(x-y)\, dy \\ &= \left(W^2_\gamma\, \tau_k\, \varphi\right)(x).\end{aligned}$$

We turn now to computing the fibers of the effective Hamiltonian $H^{(g)}_{\text{eff}}$, we notice for $x \in Q$ that

$$\left(U\, H^{(g)}_{\text{eff}}\, U^{-1}\, \varphi\right)_\xi (x) = \left(U\, h\, U^{-1}\, \varphi\right)_\xi (x) + g\left(U\, \left(W^1_\gamma - W^2_\gamma\right)\, U^{-1}\, \varphi\right)_\xi (x).$$

The fibers of the Laplace operator $-\Delta$ can be computed as follows

$$\begin{aligned}&\left[U\, (-\Delta)\, U^{-1}\, \varphi\right]_\xi (x) \\ &= \frac{1}{|\Gamma|^{1/2}} \sum_{k\in\Gamma} e^{-i(x+k)\xi}\, \left[-\Delta\, U^{-1}\, \varphi\right](x+k) \\ &= \frac{1}{|\Gamma|^{1/2}} \sum_{k\in\Gamma} e^{-i(x+k)\xi}\, (-\Delta) \left[\frac{1}{|\Gamma|^{1/2}} \sum_{\eta\in\Gamma^*} e^{i(x+k)\eta}\, \varphi_\eta(x)\right].\end{aligned}$$

Since the sum over Γ is finite and because of the linearity of $-\Delta$ we have

$$\left(U\, (-\Delta)\, U^{-1}\, \varphi\right)_\xi (x) = \frac{1}{|\Gamma|} \sum_{\eta\in\Gamma^*} \sum_{k\in\Gamma} e^{-i(x+k)(\xi-\eta)} \left[\left(\frac{1}{i}\left(\frac{d}{dx}\right) + \eta\right)^2 \varphi_\eta\right](x),$$

which implies according to Poisson's formula

$$\begin{aligned}\left(U\, (-\Delta)\, U^{-1}\, \varphi\right)_\xi (x) &= \left[\left(\frac{1}{i}\left(\frac{d}{dx}\right) + \xi\right)^2 \varphi_\xi\right](x) \\ &:= \left(-\Delta_\xi\, \varphi_\xi\right)(x). \end{aligned} \tag{4.7}$$

Moreover,

$$\begin{aligned}(U\,V\,\varphi)_\xi\,(x) &= |\Gamma|^{-1/2}\sum_{k\in\Gamma} e^{-i\xi(x+k)}\,(V\varphi)\,(x+k)\\ &= |\Gamma|^{-1/2}\sum_{k\in\Gamma} e^{-i\xi(x+k)}\,V(x+k)\,\varphi(x+k).\end{aligned}$$

Since V is Γ-periodic we conclude

$$(U\,V\,\varphi)_\xi\,(x) = V\,(U\varphi)_\xi\,(x). \tag{4.8}$$

Further using the definitions of U and W^1_γ we get

$$\begin{aligned}\left(U\,W^1_\gamma\,U^{-1}\,\varphi\right)(x,\xi) &= |\Gamma|^{-1/2}\sum_{k\in\Gamma} e^{-i\xi(x+k)}\left(W^1_\gamma\,U^{-1}\,\varphi\right)(x+k)\\ &= |\Gamma|^{-1/2}\sum_{k\in\Gamma} e^{-i\xi(x+k)}\,W^1_\gamma(x+k)\,\left(U^{-1}\,\varphi\right)(x+k).\end{aligned}$$

Since W^1_γ is Γ-periodic we get the same result as above

$$\begin{aligned}\left(U\,W^1_\gamma\,U^{-1}\,\varphi\right)(x,\xi) &= W^1_\gamma(x)\;|\Gamma|^{-1/2}\sum_{k\in\Gamma} e^{-i\xi(x+k)}\left(U^{-1}\varphi\right)(x+k)\\ &= W^1_\gamma(x)\,\varphi(x),\end{aligned}$$

which can be written as follows

$$\left(U\,W^1_\gamma\,U^{-1}\,\varphi\right)(x,\xi) = \frac{1}{|\Gamma|^{1/2}}\sum_{\eta\in\Gamma^*}\int_Q (UW)_0\,(x-y)\,\gamma_\eta(y,y)\,\varphi(x)\,dy.$$

Indeed,

$$\sum_{\eta\in\Gamma^*}\int_Q (UW)_0\,(x-y)\,\gamma_\eta(y,y)\,\varphi(x)\,dy = \sum_{\eta\in\Gamma^*}\int_Q \frac{1}{|\Gamma|^{1/2}}\sum_{k\in\Gamma} W(x-y+k)\,\gamma_\eta(y,y)\,\varphi(x)dy.$$

According to (3.15) and with Poisson's formula we find

$$\begin{aligned}&\sum_{\eta\in\Gamma^*}\int_Q (UW)_0\,(x-y)\,\gamma_\eta(y,y)\,\varphi(x)\,dy\\ &= |\Gamma|^{-1/2}\sum_{\eta\in\Gamma^*}\int_Q\sum_{k\in\Gamma} W(x-y+k)\sum_{m\in\Gamma} e^{-i(y-y+m)\eta}\,\gamma(y+m,y)\,\varphi(x)\,dy\\ &= |\Gamma|^{1/2}\int_Q\sum_{k\in\Gamma} W(x-y+k)\,\gamma(y,y)\,\varphi(x)\,dy.\end{aligned}$$

Since γ is Γ-periodic we conclude

$$\sum_{\eta\in\Gamma^*}\int\limits_Q (UW)_0\,(x-y)\,\gamma_\eta(y,y)\,\varphi(x)\,dy = |\Gamma|^{1/2}\int\limits_\Lambda W(x-y)\,\gamma(y,y)\,\varphi(x)\,dy$$
$$= |\Gamma|^{1/2}\,\left(W^1_\gamma\varphi\right)(x).$$

Furthermore, the kernel of the operator W^2_γ satisfies

$$\left(W^2_\gamma\right)^*(x,y) = W^2_\gamma(y,x),$$

since γ is a self-adjoint operator and W is real and symmetric. Therefore a similar computation as in Lemma 3.2 implies

$$\left(U\,W^2_\gamma\,U^{-1}\,\varphi\right)(x,\xi) = \int\limits_Q\sum_{k\in\Gamma} e^{-i(x-y+k)\xi}\,W^2_\gamma(x+k,y)\,\varphi(y)\,dy.$$

Using the Floquet operator U we get

$$\left(U\,W^2_\gamma\,U^{-1}\,\varphi\right)(x,\xi) = |\Gamma|^{1/2}\int\limits_Q e^{iy\xi}\left(UW^2_\gamma(.,y)\right)(x,\xi)\,\varphi(y)\,dy.$$

On the one hand

$$\left(U\,W^2_\gamma\,U^{-1}\,\varphi\right)(x,\xi) = |\Gamma|^{1/2}\int\limits_Q e^{iy\xi}\Big(U\gamma(.,y)W(.-y)\Big)(x,\xi)\,\varphi(y)\,dy$$
$$= \int\limits_Q\sum_{k\in\Gamma} e^{-i\xi(x-y+k)}\,\gamma(x+k,y)\,W(x-y+k)\,\varphi(y)\,dy.$$

On the other hand

$$\sum_{\eta\in\Gamma^*}\int\limits_Q (UW)_{\xi-\eta}\,(x-y)\,\gamma_\eta(x,y)\,\varphi(y)dy$$
$$= |\Gamma|^{-1/2}\sum_{\eta\in\Gamma^*}\int\limits_Q\sum_{k\in\Gamma} e^{-i(\xi-\eta)(x-y+k)}\,W(x-y+k)\,\gamma_\eta(x,y)\,\varphi(y)\,dy.$$

Using (3.15) we obtain

$$\sum_{\eta\in\Gamma^*}\int\limits_Q (UW)_{\xi-\eta}\,(x-y)\gamma_\eta(x,y)\varphi(y)dy$$
$$= |\Gamma|^{-1/2}\sum_{\eta\in\Gamma^*}\int\limits_Q\Bigg[\sum_{k\in\Gamma} e^{-i(\xi-\eta)(x-y+k)}\,W(x-y+k)\sum_{m\in\Gamma} e^{-i(x-y+m)\eta}\,\gamma(x+m,y)\,\varphi(y)\Bigg]\,dy.$$

Finally with Poisson's formula we deduce

$$\begin{aligned}
&\sum_{\eta\in\Gamma^*} \int_Q (UW)_{\xi-\eta}\,(x-y)\,\gamma_\eta(x,y)\,\varphi(y)\,dy \\
&= |\Gamma|^{1/2} \int_Q \sum_{k\in\Gamma} e^{-i\xi(x-y+k)}\,W(x-y+k)\,\gamma(x+k,y)\,\varphi(y)\,dy \\
&= |\Gamma|^{1/2}\,\Big(UW_\gamma^2\,U^{-1}\,\varphi\Big)_\xi\,(x).
\end{aligned}$$

□

We give now an explicit formula for the fibers of the Hamiltonian $H_N^{(g)}$ defined in (2.9) by using the second quantization [26].

Lemma 4.2. *Let*

$$H_N^{(g)} = \sum_{i=1}^{n} h_i + g\sum_{i<j} W_{i,j}$$

be a Γ*-periodic, self-adjoint operator on a dense domain* $D_N \subseteq \bigwedge_{i=1}^{N} \mathfrak{H}_\Lambda$. *Define*

$$\begin{aligned}
\Gamma(U) : \bigwedge^N \mathfrak{H}_\Lambda &\longrightarrow \bigwedge^N \mathfrak{H}_\Lambda \\
\Gamma(U) &= U\otimes\ldots\otimes U,
\end{aligned}$$

and suppose that for all $\varphi\in\mathfrak{H}_\Lambda$ *that*

$$\Big(U\,h_i\,U^{-1}\,\varphi\Big)(x,\xi) = h_{i,\xi}(x)\,\varphi(x,\xi), \tag{4.9}$$

where $h_{i,\xi} = \Big[\frac{1}{i}(\frac{d}{dx_i}) + \xi\Big]^2 + V$. *Then*

$$\left[(U\otimes U)\,W\left(U^{-1}\otimes U^{-1}\right)\psi\right](x,\xi;y,\eta) = |\Gamma|^{-1/2}\sum_{\kappa\in\Gamma^*}(UW)_\kappa\,(x-y)\psi(x,\xi-\kappa;y,\eta+\kappa),$$

for all $\psi\in\mathfrak{H}_\Lambda\otimes\mathfrak{H}_\Lambda$, *and the fibers of the Hamiltonian* $H_N^{(g)}$ *are given explicitly by*

$$\Big(H_N^{(g)}\Big)_\xi = \Gamma(U)\,h_N\,\Gamma(U)^{-1} + g\,\Gamma(U)\,W_N\,\Gamma(U)^{-1},$$

where h_N *and* W_N *are the second quantization of* h_i *and* $W_{i,j}$ *for all* $i,j\in\{1,2,\ldots,N\}$. *They are defined below in* (4.11) *and* (4.13) *respectively.*

Proof. According to the definition (3.6) of the Floquet operator U we have

$$\begin{aligned}&\left[(U\otimes U)\,W\left(U^{-1}\otimes U^{-1}\right)\varphi\right](x,\xi;y,\eta)\\&=|\Gamma|^{-1}\sum_{k,k'\in\Gamma}e^{-i\eta(y+k')}e^{-i\xi(x+k)}W(x-y+k-k')\left[\left(U^{-1}\otimes U^{-1}\right)\varphi\right](x+k;y+k').\end{aligned}$$

Using the inverse of U we get

$$\begin{aligned}&\left[(U\otimes U)\,W\left(U^{-1}\otimes U^{-1}\right)\varphi\right](x,\xi;y,\eta)\\&=|\Gamma|^{-2}\sum_{k,k'\in\Gamma}\sum_{\xi',\eta'\in\Gamma^*}e^{-i(\eta-\eta')(y+k')}\,e^{-i(\xi-\xi')(x+k)}\,W(x-y+k-k')\,\varphi(x,\xi';y,\eta').\end{aligned}$$

We multiply with the identity $e^{-i(\xi-\xi')(y+k')}\,e^{i(\xi-\xi')(y+k')}=1$ to deduce

$$\begin{aligned}&\left[(U\otimes U)\,W\left(U^{-1}\otimes U^{-1}\right)\varphi\right](x,\xi;y,\eta)\\&=|\Gamma|^{-2}\sum_{k,k'\in\Gamma}\sum_{\xi',\eta'\in\Gamma^*}e^{-i(\eta-\eta'+\xi-\xi')(y+k')}\,e^{-i(\xi-\xi')(x-y+k-k')}\,W(x-y+k-k')\,\varphi(x,\xi';y,\eta').\end{aligned}$$

Again using the unitarity of U and [[25], Thm VIII.33] we can write

$$\begin{aligned}&\left[(U\otimes U)\,W\left(U^{-1}\otimes U^{-1}\right)\varphi\right](x,\xi;y,\eta)\\&=|\Gamma|^{-3/2}\sum_{k'\in\Gamma}\sum_{\xi',\eta'\in\Gamma^*}e^{-i(\eta-\eta'+\xi-\xi')(y+k')}\,(UW)\,(x-y-k',\xi-\xi')\,\varphi(x,\xi';y,\eta').\end{aligned}$$

Since $(UW)\,(x,\xi)$ is Γ-periodic we get

$$\begin{aligned}&\left[(U\otimes U)\,W\left(U^{-1}\otimes U^{-1}\right)\varphi\right](x,\xi;y,\eta)\\&=|\Gamma|^{-3/2}\sum_{k'\in\Gamma}\sum_{\xi',\eta'\in\Gamma^*}e^{-i(\eta-\eta'+\xi-\xi')(y+k')}\,(UW)\,(x-y,\xi-\xi')\,\varphi(x,\xi';y,\eta'),\end{aligned}$$

which is owing to Poisson's formula equivalent to

$$\begin{aligned}&\left[(U\otimes U)\,W\left(U^{-1}\otimes U^{-1}\right)\varphi\right](x,\xi;y,\eta)\\&=|\Gamma|^{-1/2}\sum_{\xi',\eta'\in\Gamma^*}\delta_{\eta-\eta',\xi-\xi'}\,(UW)\,(x-y,\xi-\xi')\varphi(x,\xi';y,\eta').\end{aligned}$$

We sum over η' to get the assertion

$$\begin{aligned}&\left[(U\otimes U)\,W\left(U^{-1}\otimes U^{-1}\right)\varphi\right](x,\xi;y,\eta)\\&=|\Gamma|^{-1/2}\sum_{\xi'\in\Gamma^*}(UW)\,(x-y,\xi-\xi')\,\varphi(x,\xi';y,\eta+\xi-\xi')\\&=|\Gamma|^{-1/2}\sum_{\kappa\in\Gamma^*}(UW)\,(x-y,\kappa)\,\varphi(x,\xi-\kappa;y,\eta+\kappa).\end{aligned}$$

We have now

$$\Gamma(U) : \bigwedge^N \mathfrak{H}_\Lambda \longrightarrow \bigwedge^N \mathfrak{H}_\Lambda$$

with

$$\Gamma(U) = U \otimes \ldots \otimes U, \tag{4.10}$$

then $\Gamma(U)\, H_N^{(g)}\, \Gamma(U)^{-1}$ can be computed as follows: Let $(h_i, D) \in \mathscr{L}(\mathfrak{H}_\Lambda)$ with

$$h_i = -\Delta_{x_i} + V(x_i),$$

be a closed and densely defined operator, let moreover $\{\psi_k\}_{k\in\mathbb{N}} \subseteq D$ an orthonormal basis in $\mathfrak{H}_\Lambda$. Then we define

$$\begin{aligned} h_N : \bigotimes^N D &\longrightarrow \bigotimes^N \mathfrak{H}_\Lambda \\ h_N &:= \sum_{i=1}^N \mathbb{1} \otimes \ldots \otimes \underbrace{h_i}_{i-\text{th factor}} \otimes \ldots \otimes \mathbb{1}. \end{aligned} \tag{4.11}$$

In our case

$$h_N := \sum_{i=1}^N \Big(-\Delta_i + V(x_i)\Big).$$

Let $\psi_1, \ldots, \psi_N \in D$, then we have

$$h_N(\psi_1, \ldots, \psi_N) = \sum_{i=1}^N \psi_1 \otimes \ldots \otimes h_i\psi_i \otimes \ldots \otimes \psi_N.$$

According to (4.11) and for all $x_i \in Q$ and $\xi_i \in \Gamma^*$, $\forall i \in \{1, 2, \ldots, N\}$

$$\begin{aligned} &\Big[\Big(\Gamma(U)\, h_N\, \Gamma(U)^{-1}\Big)\,(\psi_1 \otimes \ldots \otimes \psi_N)\Big]\,(x_1, \xi_1; \ldots ; x_N, \xi_N) \\ &= \Bigg[\sum_{i=1}^N (U \otimes \ldots \otimes U)\,(\mathbb{1} \otimes \ldots \otimes h_i \otimes \ldots \otimes \mathbb{1})\,\Big(U^{-1} \otimes \ldots \otimes U^{-1}\Big)\,(\psi_1 \otimes \ldots \otimes \psi_N)\Bigg]\,(x_1, \xi_1; \ldots ; x_N, \xi_N) \\ &= \sum_{i=1}^N \Big(UU^{-1}\psi_1\Big)\,(x_1, \xi_1) \otimes \ldots \otimes \Big(Uh_iU^{-1}\psi_i\Big)\,(x_i, \xi_i) \otimes \ldots \otimes \Big(UU^{-1}\psi_N\Big)\,(x_N, \xi_N). \end{aligned}$$

With (4.9) we obtain

$$\begin{aligned} &\Big[\Big(\Gamma(U)\, h_N\, \Gamma(U)^{-1}\Big)\,(\psi_1 \otimes \ldots \otimes \psi_N)\Big]\,(x_1, \xi_1; \ldots ; x_N, \xi_N) \\ &= \sum_{i=1}^N \psi_1(x_1, \xi_1) \otimes \ldots \otimes (h_{i,\xi}\psi_i)\,(x_i, \xi_i) \otimes \ldots \otimes \psi_N(x_N, \xi_N). \end{aligned} \tag{4.12}$$

Let now $W_N : \overset{N}{\bigotimes}\mathfrak{H}_\Lambda \longrightarrow \overset{N}{\bigotimes}\mathfrak{H}_\Lambda$ with

$$W_N := \sum_{i<j} \prod_{i,j} (W \otimes \mathbb{1} \otimes \mathbb{1} \cdots \otimes \mathbb{1}) \prod_{i,j}, \tag{4.13}$$

where the permutation operator $\prod_{i,j} = \prod_{i,j}^{-1} \in \mathscr{B}\Big(\overset{N}{\bigotimes}\mathfrak{H}_\Lambda\Big)$ is defined by

$$\prod_{i,j}(\psi_1, \ldots, \psi_N) = \psi_i \otimes \psi_j \otimes \ldots \otimes \psi_{i-1} \otimes \psi_1 \otimes \psi_{i+1} \otimes \ldots \otimes \psi_{j-1} \otimes \psi_2 \otimes \psi_{j+1} \otimes \ldots \otimes \psi_N \tag{4.14}$$

for $i, j \in \{1, 2, \ldots, N\}$ with $N \in \mathbb{N}$, $N \geq 2$ and for all $\psi_1, \ldots, \psi_N \in \mathfrak{H}_\Lambda$. Since

$$(W\psi)(x, y) = W(x - y)\, \psi(x, y),$$

for $\psi \in \mathfrak{H}_\Lambda \times \mathfrak{H}_\Lambda$, then we have

$$W_N(x_1, x_2, \ldots, x_N) = \sum_{i<j} W(x_i - x_j).$$

Moreover, we notice that the permutation operator commutes with the unitary operator $\Gamma(U)$, i.e., $\big[\Gamma(U), \prod_{i,j}\big] = 0$. Indeed, for $\psi_1, \ldots, \psi_N \in \mathfrak{H}_\Lambda$ we have

$$\begin{aligned}
&\left[\Gamma(U) \prod_{i,j}\right] (\psi_1 \otimes \ldots \otimes \psi_N] \\
&= \Gamma(U)\big(\psi_i \otimes \psi_j \otimes \ldots \otimes \psi_{i-1} \otimes \psi_1 \otimes \psi_{i+1} \otimes \ldots \otimes \psi_{j-1} \otimes \psi_2 \otimes \psi_{j+1} \otimes \ldots \otimes \psi_N\big) \\
&= U\psi_i \otimes U\psi_j \otimes \ldots \otimes U\psi_N \\
&= \prod_{i,j} \Gamma(U)\, (\psi_1 \otimes \ldots \otimes \psi_N)\, .
\end{aligned}$$

Similarly we get $\big[\Gamma(U)^{-1}, \prod_{i,j}\big] = 0$. Together with (4.13) and for all $x_i \in Q$ and $\xi_i \in \Gamma^*$, $\forall i \in \{1, 2, \ldots, N\}$ we can write

$$\begin{aligned}
&\big[\Gamma(U)\, W_N\, \Gamma(U)^{-1}(\psi_1 \otimes \ldots \otimes \psi_N)\big]\, (x_1, \xi_1; \ldots; x_N, \xi_N) \\
&= \left[\sum_{i<j} \Gamma(U) \prod_{i,j} (W \otimes \mathbb{1} \otimes \ldots \otimes \mathbb{1}) \prod_{i,j} \Gamma(U)^{-1}(\psi_1 \otimes \ldots \otimes \psi_N)\right] (x_1, \xi_1; \ldots; x_N, \xi_N) \\
&= \left[\sum_{i<j} \prod_{i,j} \Gamma(U)\, (W \otimes \mathbb{1} \otimes \ldots \otimes \mathbb{1})\Gamma(U)^{-1} \prod_{i,j}(\psi_1 \otimes \ldots \otimes \psi_N)\right] (x_1, \xi_1; \ldots; x_N, \xi_N).
\end{aligned}$$

With (4.10) and (4.14) we obtain

$$\begin{aligned}
&\big[\Gamma(U)\, W_N\, \Gamma(U)^{-1}(\psi_1 \otimes \ldots \otimes \psi_N)\big]\, (x_1, \xi_1; \ldots; x_N, \xi_N) \\
&= \left[\sum_{i<j} \prod_{i,j} \Big\{ \big((U \otimes U)\, W\, (U^{-1} \otimes U^{-1})\psi_i \otimes \psi_j\big) \otimes \ldots \otimes \psi_N) \Big\}\right] (x_1, \xi_1; \ldots; x_N, \xi_N),
\end{aligned}$$

which is according to (4.9) equivalent to

$$\begin{aligned}&\left[\Gamma(U)\, W_N\, \Gamma(U)^{-1}(\psi_1 \otimes \ldots \otimes \psi_N)\right](x_1,\xi_1;\ldots;x_N,\xi_N) = \sum_{i<j}\Big[\psi_1(x_1,\xi_1)\otimes\ldots\\ &\ldots\otimes\Big(|\Gamma|^{-1/2}\sum_{\kappa\in\Gamma^*}(UW)(x_i-y_i,\kappa_i)\psi_i(x_i,\xi_i-\kappa_i)\otimes\psi_j(x_j,\eta_j+\kappa_j)\Big)\otimes\ldots\otimes\psi_N(x_N,\xi_N)\Big]. \qquad (4.15)\end{aligned}$$

From (4.12) and (4.15) we conclude

$$\left(H_N^{(g)}\right)_\xi = \Gamma(U)\, H_N^{(g)}\, \Gamma(U)^{-1}\Gamma(U)\, h_N\, \Gamma(U)^{-1} + g\,\Gamma(U)\, W_N\, \Gamma(U)^{-1}.$$

□

4.2 Lieb's Variational Principle: Periodic Case

In this section Lieb's variational principle will be generalized by using the fibers of the HF functional, which will be computed explicitly in the following lemma.

Lemma 4.3. *For all* Γ*-periodic, self-adjoint operators* $\gamma \in \mathscr{L}^1(\mathfrak{H}_\Lambda)$*, the HF functional* (4.1) *can be written as follows*

$$\begin{aligned}\mathcal{E}_{\mathrm{hf}}(\gamma) = &\sum_{\xi\in\Gamma^*}\mathrm{Tr}_{\mathfrak{H}_Q}\{h_\xi\gamma_\xi\} + \frac{g}{2\,|\Gamma|^{\frac{1}{2}}}\sum_{\eta,\xi\in\Gamma^*}\int_Q\int_Q\Big\{(UW)_0(x-y)\gamma_\xi(x,x)\gamma_\eta(y,y)\\ &- (UW)_{\xi-\eta}(x-y)\gamma_\xi(x,y)\overline{\gamma_\eta(x,y)}\Big\}dxdy, \qquad (4.16)\end{aligned}$$

where

$$h_\xi := -\Delta_\xi + V = \left(\frac{1}{i}\left(\frac{d}{dx}\right)+\xi\right)^2 + V.$$

Before we begin with the proof of this lemma we give some remarks about the Floquet operator U.

Remark 4.1. 1. For all $f \in \mathfrak{H}_\Lambda$ we have

$$\begin{aligned}(Uf)_\xi(x) &= \frac{1}{|\Gamma|^{1/2}}\sum_{k\in\Gamma}e^{-i\xi(x+k)}f(x+k)\\ &= e^{-i\xi x}\,\mathcal{F}\Big[f(x+.)\Big](\xi),\end{aligned}$$

Then for $f \cdot g \in \mathfrak{H}_\Lambda$ we can write

$$\begin{aligned}(U\, f\, g)_\xi\,(x) &= \frac{1}{|\Gamma|^{1/2}} \sum_{k\in\Gamma} e^{-i\xi(x+k)}\, f(x+k)\, g(x+k)\\ &= e^{-i\xi x}\, \mathcal{F}\Big[f\, g(x+.)\Big](\xi),\end{aligned}$$

using the Fourier transform of a multiplication of functions we obtain

$$\begin{aligned}(U\, f\, g)_\xi\,(x) &= \frac{e^{-i\xi x}}{|\Gamma|^{1/2}} \Big\{\mathcal{F}\Big[f(x+.)\Big] \underset{\xi}{\star} \mathcal{F}\Big[(g(x+.)\Big]\Big\}(\xi)\\ &= \frac{1}{|\Gamma|^{1/2}} \sum_{\eta\in\Gamma^*} e^{-i\xi x}\, \mathcal{F}\Big[f(x+.)\Big](\xi-\eta)\, \mathcal{F}\Big[g(x+.)\Big](\eta)\\ &= \frac{1}{|\Gamma|^{1/2}} \sum_{\eta\in\Gamma^*} e^{-i(\xi-\eta)x} \mathcal{F}\Big[f(x+.)\Big](\xi-\eta)\, e^{-i\eta x}\, \mathcal{F}\Big[g(x+.)\Big](\eta)\\ &= \frac{1}{|\Gamma|^{1/2}} \sum_{\eta\in\Gamma^*} (Uf)_{\xi-\eta}\,(x)\;(Ug)_\eta\,(x),\end{aligned}$$

where $f \underset{\xi}{\star} g$ denotes the convolution of f and g with respect to $\xi \in \Gamma^*$. Thus, for all $f_1 \otimes f_2, g_1 \otimes g_2 \in \mathfrak{H}_\Lambda \otimes \mathfrak{H}_\Lambda$ we can write

$$\begin{aligned}&[(U\otimes U)\,(f_1\otimes f_2)\,(g_1\otimes g_2)]\,(x,\xi;y,\eta)\\ &= [(U f_1\, g_1)\otimes(U f_2\, g_2)]\,(x,\xi;y,\eta)\\ &= \frac{1}{|\Gamma|}\,\Big[(Uf_1)_\xi \underset{\xi}{\star} (Ug_1)_\xi\Big]\,(x)\,\Big[(Uf_2)_\eta \underset{\eta}{\star} (Ug_2)_\eta\Big]\,(y)\\ &= \frac{1}{|\Gamma|} \sum_{\xi',\eta'\in\Gamma^*} (Uf_1)_{\xi-\xi'}\,(x)\,(Uf_2)_{\eta-\eta'}\,(y)\,(Ug_1)_{\xi'}\,(y)\,(Ug_2)_{\eta'}\,(y)\\ &= \frac{1}{|\Gamma|}\,\Big[(U\otimes U)\,(f_1\otimes f_2)\Big] \underset{\xi,\eta}{\star} \Big[(U\otimes U)\,(g_1\otimes g_2)\Big](x,y).\end{aligned}$$

2. According to the last equation we can write for any operator A defined on $\mathfrak{H}_\Lambda \otimes \mathfrak{H}_\Lambda$ that

$$(U\otimes U)\,A\,\Big(U^{-1}\otimes U^{-1}\Big)\,\varphi = \frac{1}{|\Gamma|}\;[(U\otimes U)\,A] \underset{\xi,\eta}{*} \varphi. \tag{4.17}$$

Proof of Lemma 4.3: Using the definition (3.6) of the unitary operator U we obtain

$$\begin{aligned}
\mathcal{E}_{\mathrm{hf}}(\gamma) &= \mathrm{Tr}_{\mathfrak{H}_\Lambda}\{h\,\gamma\} + \frac{g}{2}\,\mathrm{Tr}_{\mathfrak{H}_\Lambda\otimes\mathfrak{H}_\Lambda}\{W(1-\mathrm{Ex})(\gamma\otimes\gamma)\} \\
&= \mathrm{Tr}_{\widetilde{\mathfrak{H}}_\Lambda}\{U\,h\,U^{-1}\,U\,\gamma\,U^{-1}\} \\
&\quad + \frac{g}{2}\,\mathrm{Tr}_{\widetilde{\mathfrak{H}}_\Lambda\otimes\widetilde{\mathfrak{H}}_\Lambda}\{(U\otimes U)\;W\;\left(U^{-1}\otimes U^{-1}\right)(U\otimes U)\,(1-\mathrm{Ex})(\gamma\otimes\gamma)\,\left(U^{-1}\otimes U^{-1}\right)\},
\end{aligned}$$

since $U\otimes U$ commutes with $(1-\mathrm{Ex})$ we get

$$\mathcal{E}_{\mathrm{hf}}(\gamma) = \mathrm{Tr}_{\widetilde{\mathfrak{H}}_\Lambda}\{\widetilde{h}\,\widetilde{\gamma}\} + \frac{g}{2}\,\mathrm{Tr}_{\widetilde{\mathfrak{H}}_\Lambda\otimes\widetilde{\mathfrak{H}}_\Lambda}\left\{\widetilde{W}(1-\mathrm{Ex})\widetilde{\gamma}\otimes\widetilde{\gamma}\right\}, \tag{4.18}$$

where

$$\begin{aligned}
\widetilde{h} &:= U\,h\,U^{-1}, \\
\widetilde{\gamma} &:= U\,\gamma\,U^{-1} \\
\widetilde{W} &:= (U\otimes U)\,W\left(U^{-1}\otimes U^{-1}\right).
\end{aligned}$$

But according to (4.7) and (4.8) we have

$$\mathrm{Tr}_{\widetilde{\mathfrak{H}}_\Lambda}\left\{\widetilde{h}\,\widetilde{\gamma}\right\} = \sum_{\xi\in\Gamma^*}\mathrm{Tr}_{\mathfrak{H}_Q}\left\{h_\xi\,\gamma_\xi\right\}.$$

Moreover, to compute the second term in (4.18) we must first find the integral kernel of the operator $\widetilde{\gamma}\otimes\widetilde{\gamma}$. We notice

$$\begin{aligned}
&[(\widetilde{\gamma}\otimes\widetilde{\gamma})\,(f\otimes g)]\,(x,\xi;y,\eta) \\
&= (\widetilde{\gamma}f)\,(x,\xi)\otimes(\widetilde{\gamma}g)\,(y,\eta) \\
&= \left(\sum_{\xi'\in\Gamma^*}\int_Q \widetilde{\gamma}(x,\xi;x',\xi')f(x',\xi')dx'\right)\left(\sum_{\eta'\in\Gamma^*}\int_Q \widetilde{\gamma}(y,\eta;y',\eta')g(y',\eta')dy'\right).
\end{aligned}$$

Using Lemma 3.3 we obtain

$$\begin{aligned}
&[(\widetilde{\gamma}\otimes\widetilde{\gamma})\,(f\otimes g)]\,(x,\xi;y,\eta) \\
&= \left(\sum_{\xi'\in\Gamma^*}\int_Q \gamma_\xi(x,x')\,\delta_{\xi,\xi'}\,f(x',\xi')\,dx'\right)\left(\sum_{\eta'\in\Gamma^*}\int_Q \gamma_\eta(y,y')\,\delta_{\eta,\eta'}\,g(y',\eta')dy'\right) \\
&= \sum_{\xi',\eta'\in\Gamma^*}\int_Q\int_Q\Big[\left(\gamma_\xi(x,x')\,\delta_{\xi,\xi'}\,\gamma_\eta(y,y')\,\delta_{\eta,\eta'}\right)(f\otimes g)\Big](x',\xi';y',\eta')\,dx'\,dy'.
\end{aligned}$$

Thus, the integral kernel of $\widetilde{\gamma} \otimes \widetilde{\gamma}$ is given by

$$(\widetilde{\gamma} \otimes \widetilde{\gamma})\,(x, \xi; y, \eta) = \sum_{\xi', \eta' \in \Gamma^*} \int_Q \int_Q \gamma_\xi(x, x')\, \delta_{\xi,\xi'}\, \gamma_\eta(y, y')\, \delta_{\eta,\eta'}\, dx'\, dy'. \tag{4.19}$$

Further, the definition (3.6) of U gives

$$\begin{aligned}
&[(U \otimes U)\, W]\,(x, \xi; y, \eta) \\
&= \frac{1}{|\Gamma|^{1/2}} \sum_{l \in \Gamma} e^{-i\eta(y+l)} \left[\frac{1}{|\Gamma|^{1/2}} \sum_{k \in \Gamma} e^{-i\xi(x+k)}\, W(x + k - y - l) \right] \\
&= \frac{1}{|\Gamma|^{1/2}} \sum_{l \in \Gamma} e^{-i\eta(y+l)} e^{-i\xi l} \left[\frac{1}{|\Gamma|^{1/2}} \sum_{k \in \Gamma} e^{-i\xi(x+k-l)}\, W(x + k - y - l) \right].
\end{aligned}$$

The Poisson's formula now implies

$$\begin{aligned}
[(U \otimes U)\, W]\,(x, \xi; y, \eta) &= |\Gamma|^{1/2}\, \delta_{\xi+\eta,0}\, (UW)_\xi\, (x - y - l) \\
&= |\Gamma|^{1/2}\, \delta_{\xi+\eta,0}\, (UW)_\xi\, (x - y),
\end{aligned} \tag{4.20}$$

where the periodicity of $(UW)_\xi$ with respect to Γ is used in the last equation. Applying (4.17) and (4.20) yield

$$\begin{aligned}
&\left[\widetilde{W}\,(U \otimes U)\,(f \otimes g)\right](x, \xi; y, \eta) \\
&= \frac{1}{|\Gamma|} \sum_{\xi', \eta' \in \Gamma^*} [(U \otimes U)\, W]\,(x, \xi - \xi'; y, \eta - \eta')\,(Uf)\,(x, \xi')\,(Ug)\,(y, \eta') \\
&= \frac{1}{|\Gamma|^{1/2}} \sum_{\xi', \eta' \in \Gamma^*} \delta_{\xi-\xi', \eta'-\eta}\, (UW)_{\xi-\xi'}\,(x - y)\,(Uf)\,(x, \xi')\,(Ug)\,(y, \eta') \\
&= \frac{1}{|\Gamma|^{1/2}} \sum_{\xi' \in \Gamma^*} (UW)_{\xi-\xi'}\,(x - y)\,(Uf)\,(x, \xi')\,(Ug)\,(y, \eta + \xi - \xi') \\
&= \frac{1}{|\Gamma|^{1/2}} \sum_{\kappa \in \xi - \Gamma^*} (UW)_\kappa\,(x - y)\,(Uf)\,(x, \xi - \kappa)\,(Ug)\,(y, \eta + \kappa),
\end{aligned}$$

since $\Gamma^* = \frac{2\pi}{L}\,\Lambda_\ell$ and $\xi \in \Gamma^*$, then $\xi - \Gamma^* = \Gamma^*$. Now the last equation allows us to write

$$\begin{aligned}
&\left[\widetilde{W}\,(\widetilde{\gamma} \otimes \widetilde{\gamma})\,(f \otimes g)\right](x, \xi; y, \eta) \\
&= \left[\widetilde{W}\,(\widetilde{\gamma} f \otimes \widetilde{\gamma} g)\right](x, \xi; y, \eta) \\
&= \frac{1}{|\Gamma|^{1/2}} \sum_{\kappa \in \xi - \Gamma^*} (UW)_\kappa\,(x - y)\,(\widetilde{\gamma} f \otimes \widetilde{\gamma} g)\,(x, \xi - \kappa; y, \eta + \kappa),
\end{aligned}$$

which according to (4.19) equivalent to

$$\left[\widetilde{W}\left(\widetilde{\gamma}\otimes\widetilde{\gamma}\right)\left(f\otimes g\right)\right](x,\xi;y,\eta)=\frac{1}{|\Gamma|^{1/2}}\sum_{\kappa\in\Gamma^*}\left(UW\right)_\kappa(x-y)$$
$$\sum_{\xi',\eta'\in\Gamma^*}\int_Q\int_Q\left[\left(\gamma_{\xi-\kappa}(x,x')\delta_{\xi-\kappa,\xi'}\gamma_{\eta+\kappa}(y,y')\delta_{\eta+\kappa,\eta'}\right)(f\otimes g)\right](x',\xi';y',\eta')dx'dy'.$$

Therefore,

$$\begin{aligned}&\operatorname{Tr}\left\{\widetilde{W}\left(\widetilde{\gamma}\otimes\widetilde{\gamma}\right)\right\}\\&=\frac{1}{|\Gamma|^{1/2}}\sum_{\xi,\eta\in\Gamma^*}\int_Q\int_Q\sum_{\kappa\in\Gamma^*}\left(UW\right)_\kappa(x-y)\Big(\gamma_{\xi-\kappa}(x,x)\,\delta_{\xi-\kappa,\xi}\,\gamma_{\eta+\kappa}(y,y)\,\delta_{\eta+\kappa,\eta}\Big)\,dx\,dy\\&=\frac{1}{|\Gamma|^{1/2}}\sum_{\xi,\eta\in\Gamma^*}\int_Q\int_Q\left(UW\right)_0(x-y)\gamma_\xi(x,x)\,\gamma_\eta(y,y)\,dx\,dy.\end{aligned}$$

Similarly, for the exchange term we can write

$$\begin{aligned}&\left[\widetilde{W}\operatorname{Ex}\left(\widetilde{\gamma}\otimes\widetilde{\gamma}\right)\left(f\otimes g\right)\right](x,\xi;y,\eta)\\&=\left[\widetilde{W}\left(\widetilde{\gamma}g\otimes\widetilde{\gamma}f\right)\right](x,\xi;y,\eta)\\&=\frac{1}{|\Gamma|^{1/2}}\sum_{\kappa\in\xi-\Gamma^*}\left(UW\right)_\kappa(x-y)\left(\widetilde{\gamma}g\otimes\widetilde{\gamma}f\right)(x,\xi-\kappa;y,\eta+\kappa).\end{aligned}$$

According to (4.19) we obtain

$$\left[\widetilde{W}\operatorname{Ex}\left(\widetilde{\gamma}\otimes\widetilde{\gamma}\right)\left(f\otimes g\right)\right](x,\xi;y,\eta)=\frac{1}{|\Gamma|^{1/2}}\sum_{\kappa\in\Gamma^*}\left(UW\right)_\kappa(x-y)$$
$$\sum_{\xi',\eta'\in\Gamma^*}\int_Q\int_Q\Big[\Big(\gamma_{\xi-\kappa}(x,y')\,\delta_{\xi-\kappa,\eta'}\,\gamma_{\eta+\kappa}(y,x')\,\delta_{\eta+\kappa,\xi'}\Big)(f\otimes g)\Big](x',\xi';y',\eta')dx'dy'.$$

Hence,

$$\operatorname{Tr}\left\{\widetilde{W}\operatorname{Ex}\left(\widetilde{\gamma}\otimes\widetilde{\gamma}\right)\right\}=\frac{1}{|\Gamma|^{1/2}}\sum_{\xi,\eta\in\Gamma^*}\int_Q\int_Q\left(UW\right)_{\xi-\eta}(x-y)\gamma_\xi(y,x)\gamma_\eta(x,y).$$

Let us now return to Lieb's variational principle in the periodic case, which corresponds to the result in [1].

Theorem 4.1 (Lieb's variational principle)**.** *Let $N\in\mathbb{N}$, $P_{\mathrm{per}}^{(N)}$ defined in* (1.11) *and $\gamma\in P_{\mathrm{per}}^{(N)}$ such that $\gamma\neq\gamma^2$. Then $\exists\,\tilde{\gamma}\in P_{\mathrm{per}}^{(N)}$ such that $\tilde{\gamma}=\tilde{\gamma}^2$ and*

$$\mathcal{E}_{\mathrm{hf}}\left(\tilde{\gamma}\right)<\mathcal{E}_{\mathrm{hf}}(\gamma)\,.$$

Proof. We consider the fiber decomposition

$$\gamma_\xi = \sum_{j\geq 1} \mu_{\xi,j} \left|\varphi_{\xi,j}\right\rangle\!\left\langle\varphi_{\xi,j}\right|, \; \forall \xi \in \Gamma^*,$$

where $\langle \varphi_{\xi,i}|\varphi_{\xi,j}\rangle = \delta_{i,j}$, $0 \leq \mu_{\xi,j} \leq 1$ and $\sum\limits_{\xi} \sum\limits_{j\geq 1} \mu_{\xi,j} = N$. Since γ is not a projection, there exist $\sigma, \kappa \in \Gamma^*$ and $j, k \in \mathbb{N}$ with $(\sigma, j) \neq (\kappa, k)$ such that

$$0 < \mu_{\sigma,j},\, \mu_{\kappa,k} < 1,$$

We may assume without loss of generality that

$$t_{\kappa,k} \leq t_{\sigma,j}, \tag{4.21}$$

where

$$\begin{aligned} t_{\kappa,k} &:= \left\langle H_\kappa^{(g)} \right\rangle_{\varphi_{\kappa,k}} \\ &= \int\limits_Q \int\limits_Q \overline{\varphi_{\kappa,k}(x)} \left[h_\kappa(x,y) + \frac{g}{|\Gamma|^{\frac{1}{2}}} \sum_{\eta \in \Gamma^*} \left\{ (UW)_0\,(x-y)\gamma_\eta(y,y) - (UW)_{\kappa-\eta}\,(x-y)\gamma_\eta(x,y) \right\} \right] \varphi_{\kappa,k}(y)\, dx\, dy. \end{aligned} \tag{4.22}$$

Let $\rho := \min\left\{\mu_{\sigma,j}, 1-\mu_{\kappa,k}\right\} > 0$ and define

$$\gamma^\rho := U^{-1} \Big(\bigoplus_{\xi \in \Gamma^*} \gamma_\xi^\rho \Big) U,$$

such that

$$\forall \xi \neq \sigma, \kappa : \gamma_\xi^\rho = \gamma_\xi,$$

and for $\xi = \sigma$ or $\xi = \kappa$ we define

$$\begin{aligned} \gamma_\sigma^\rho &= \sum_{\substack{m\geq 1 \\ m\neq j}} \mu_{\sigma,m} \left|\varphi_{\sigma,m}\right\rangle\!\left\langle\varphi_{\sigma,m}\right| + (\mu_{\sigma,j} - \rho) \left|\varphi_{\sigma,j}\right\rangle\!\left\langle\varphi_{\sigma,j}\right| \\ \gamma_\kappa^\rho &= \sum_{\substack{n\geq 1 \\ k\neq n}} \mu_{\kappa,n} \left|\varphi_{\kappa,n}\right\rangle\!\left\langle\varphi_{\kappa,n}\right| + (\mu_{\kappa,k} + \rho) \left|\varphi_{\kappa,k}\right\rangle\!\left\langle\varphi_{\kappa,k}\right|. \end{aligned}$$

Therefore we can write

$$\gamma^\rho = U^{-1} \left[\bigoplus_{\xi \in \Gamma^*} \Big(\gamma_\xi - \delta_{\xi,\sigma}\, \rho\, \left|\varphi_{\sigma,j}\right\rangle\!\left\langle\varphi_{\sigma,j}\right| + \delta_{\xi,\kappa}\, \rho\, \left|\varphi_{\kappa,k}\right\rangle\!\left\langle\varphi_{\kappa,k}\right| \Big) \right] U.$$

For simplicity we denote

$$P_{\sigma,j} := |\varphi_{\sigma,j}\rangle\langle\varphi_{\sigma,j}|\,.$$

Then

$$\begin{aligned}
&\mathcal{E}_{\mathrm{hf}}(\gamma^{\rho}) - \mathcal{E}_{\mathrm{hf}}(\gamma) = -\rho\,\langle\varphi_{\sigma,j}|h_\sigma\varphi_{\sigma,j}\rangle + \rho\,\langle\varphi_{\kappa,k}|h_\kappa\varphi_{\kappa,k}\rangle\\
&+ \frac{g}{2\,|\Gamma|^{\frac{1}{2}}}\sum_{\eta,\xi\in\Gamma^*}\int_Q\int_Q (UW)_0(x-y)\Big\{M_\xi(x,x)\,M_\eta(y,y) - \gamma_\xi(x,x)\,\gamma_\eta(y,y)\Big\}\,dx\,dy\\
&- \frac{g}{2\,|\Gamma|^{\frac{1}{2}}}\sum_{\eta,\xi\in\Gamma^*}\int_Q\int_Q (UW)_{\xi-\eta}(x-y)\Big\{M_\xi(x,y)\,\overline{M_\eta(x,y)} - \gamma_\xi(x,y)\,\overline{\gamma_\eta(x,y)}\Big\}\,dx\,dy,
\end{aligned}$$

where

$$M_\xi(x,y) := \gamma_\xi\,(x,y) - \rho\,\delta_{\xi,\sigma}\,P_{\sigma,j}(x,y) + \rho\,\delta_{\xi,\kappa}\,P_{\kappa,k}(x,y).$$

In terms of ρ as a common factor we deduce

$$\begin{aligned}
&\mathcal{E}_{\mathrm{hf}}(\gamma^{\rho}) - \mathcal{E}_{\mathrm{hf}}(\gamma) = \rho\Big\{-\langle\varphi_{\sigma,j}|\,h_\sigma\,\varphi_{\sigma,j}\rangle + \langle\varphi_{\kappa,k}|\,h_\kappa\,\varphi_{\kappa,k}\rangle\\
&+ \frac{g}{2\,|\Gamma|^{\frac{1}{2}}}\sum_{\eta,\xi\in\Gamma^*}\int_Q\int_Q\Big[(UW)_0\,(x-y)\,\big[-2\,\delta_{\xi,\sigma}\,P_{\sigma,j}(x,x)\,\gamma_\eta(x,x)\,+2\delta_{\xi,\kappa}\,P_{k,\kappa}(y,y)\,\gamma_\eta(y,y)\big]\\
&- \mathrm{Re}\Big((UW)_{\xi-\eta}(x-y)\big[-2\,\delta_{\xi,\sigma}\,P_{\sigma,j}(x,y)\,\overline{\gamma_\eta(x,y)} + 2\,\delta_{\xi,\kappa}\,P_{k,\kappa}(x,y)\,\overline{\gamma_\eta(x,y)}\big]\Big)\Big]\,dx\,dy\Big\}\\
&- R\,\rho^2.
\end{aligned}$$

According to the Kronecker-delta we have

$$\begin{aligned}
&\mathcal{E}_{\mathrm{hf}}(\gamma^{\rho}) - \mathcal{E}_{\mathrm{hf}}(\gamma) = \rho\Big\{-\langle\varphi_{\sigma,j}|\,h_\sigma\,\varphi_{\sigma,j}\rangle + \langle\varphi_{\kappa,k}|\,h_\kappa\,\varphi_{\kappa,k}\rangle\\
&+ \frac{g}{|\Gamma|^{\frac{1}{2}}}\sum_{\eta\in\Gamma^*}\int_Q\int_Q\Big[(UW)_0\,(x-y)\,\Big(\big|\varphi_{\kappa,k}(x)\big|^2 - |\varphi_{\sigma,j}(x)|^2\Big)\,\gamma_\eta(y,y)\\
&- \mathrm{Re}\Big((UW)_{\kappa-\eta}\,(x-y)\varphi_{\kappa,k}(x)\,\overline{\varphi_{\kappa,k}(y)}\,\overline{\gamma_\eta(x,y)} - (UW)_{\sigma-\eta}\,(x-y)\,\varphi_{\sigma,j}(x)\,\overline{\varphi_{\sigma,j}(y)}\,\overline{\gamma_\eta(x,y)}\Big)\Big]\,dx\,dy\Big\}\\
&- R\,\rho^2.
\end{aligned}$$

Which is equivalent to

$$\mathcal{E}_{\mathrm{hf}}(\gamma^{\rho}) - \mathcal{E}_{\mathrm{hf}}(\gamma) = -R\rho^2 - \rho\left\{\left\langle H^{(g)}_\sigma\right\rangle_{\varphi_{\sigma,j}} - \left\langle H^{(g)}_\kappa\right\rangle_{\varphi_{\kappa,k}}\right\},$$

where $H^{(g)}_\kappa$ is the operator defined in (4.6) and its expectation value evaluated in a state $\varphi_{\kappa,k}$ is given (4.22). According to our choice of ρ and to the assumption (4.21) we deduce

$$\mathcal{E}_{\mathrm{hf}}(\gamma^{\rho}) - \mathcal{E}_{\mathrm{hf}}(\gamma) < 0.$$

It is clear that $\mathrm{rank}\,(\gamma^\rho) < \mathrm{rank}\,(\gamma)$ and owing to the fact that $\mathrm{rank}\,(\gamma) < \infty$ we obtain after finite iterations of this procedure a 1-pdm $\tilde{\gamma}$ which satisfies the assertion. $\square$

4.3 Gap Estimate for the Fiber Energy Levels

In Theorem 2.1 we have shown that if the minimization problem defined by (1.14), (1.15) and (1.17) admits a periodic minimizer, then the N first energy levels of the corresponding effective Hamiltonian are filled and the minimizer can be written as a function of $H_{\text{eff}}^{(g)}$, i.e.,

$$\gamma_{\text{per}} = \mathbb{1}\left[H_{\text{eff}}^{(g)}(\gamma_{\text{per}}) \leq e_N\right].$$

Moreover, in [34] it was shown that there is a gap in the spectrum of $H_{\text{eff}}^{(g)}$ above the N^{th} energy level. Therefore, we are interested in finding an estimate for the gap in the spectrum of $H_\xi^{(g)}\left(\gamma_{\text{per}}\right)$ above the energy level number N_ξ, where N_ξ denotes the number of the eigenvalues of $H_\xi^{(g)}\left(\gamma_{\text{per}}\right)$ below e_N, i.e.,

$$N_\xi = \#\left\{\sigma\left(H_\xi^{(g)}\left(\gamma_{\text{per}}\right)\right) \cap (-\infty, e_N]\right\} \tag{4.23}$$

and to know if this gap increases in the presence of a weak positive periodic potential. First we recall from [34] that in an exact, unrestricted HF calculation each energy level of the HF equation is either completely filled or completely empty with the assumption that the two-body interaction W is repulsive. This in turn implies the existence of a gap between the N^{th} and $(N+1)^{\text{st}}$ eigenvalues of the effective Hamiltonian. In particular, it holds

$$e_{N+1} - e_N \geq W_{N,N+1}, \tag{4.24}$$

where $W_{N,N+1}$ is given by

$$W_{N,N+1} = \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \frac{1}{2}\,\left|\varphi_{N+1}(x)\varphi_N(y) - \varphi_N(x)\varphi_{N+1}(y)\right|^2 W(x-y)\,dx\,dy.$$

Since the effective Hamiltonian $H_{\text{eff}}^{(g)}$ is Γ-periodic, it follows from Lemma 3.2 that

$$H_{\text{eff}}^{(g)} = U^{-1}\left(\bigoplus_{\xi\in\Gamma^*} H_\xi^{(g)}\right)U,$$

and using the unitarity of U, it holds

$$\sigma\left(H_{\text{eff}}^{(g)}\right) = \bigcup_{\xi\in\Gamma^*}\sigma\left(H_\xi^{(g)}\right).$$

Then, it follows from the gap estimate (4.24) on the effective Hamiltonian $H_{\text{eff}}^{(g)}$ that

$$e_{\xi,N_\xi+1} - e_{\xi,N_\xi} \geq W_{N,N+1} \tag{4.25}$$

where $(e_{\xi,j})_{j\geq 1}$ are the eigenvalues of $H_\xi^{(g)}$. However, in what follows we give a fiber dependent lower bound on the difference $e_{\xi,N_\xi+1} - e_{\xi,N_\xi}$ which improves (4.25). An argument in the same spirit of the proof of Lemma 4.3 allows us to state our gap estimate on the fiber effective Hamiltonian.

Theorem 4.2. *Let $H_{\text{eff}}^{(g)}$ be the self-adjoint operator defined in (4.5) where γ_{per} is a minimizer of $\mathcal{E}_{\text{hf}}$, $(e_{\xi,j})_{j\geq 1}$ be the eigenvalues of its fiber $H_\xi^{(g)}$ corresponding to the eigenvectors $(\varphi_{\xi,j})_{j\geq 1}$, $\forall \xi \in \Gamma^*$. Then the following gap estimate holds for all $\xi \in \Gamma^*$*

$$e_{\xi,N_\xi+1} - e_{\xi,N_\xi} \geq \frac{g}{|\Gamma|^{\frac{1}{2}}} \int_Q \int_Q (UW)_0(x-y) \left| \left(\varphi_{\xi,N_\xi} \wedge \varphi_{\xi,N_\xi+1} \right)(x,y) \right|^2 dx\, dy,$$

where the number N_ξ is defined in (4.23) and $f \wedge g = \frac{1}{\sqrt{2}}\Big(f \otimes g - g \otimes f\Big)$ for all $f, g \in \mathfrak{H}_Q$.

Proof. We recall that γ_{per} denotes a solution to the minimization problem (1.14), (1.15) and (1.17). We pick $\sigma \in \Gamma^*$ and set

$$\widetilde{\gamma} = U^{-1} \left(\bigoplus_{\xi \in \Gamma^*} \widetilde{\gamma_\xi} \right) U,$$

such that $\widetilde{\gamma_\xi} = (\gamma_{\text{per}})_\xi$, $\forall \xi \neq \sigma$ and

$$\begin{aligned} \widetilde{\gamma}_\sigma :&= \sum_{j=1}^{N_\sigma - 1} |\varphi_{\sigma,j}\,\rangle\langle\, \varphi_{\sigma,j}| + |\varphi_{\sigma,N_\sigma+1}\,\rangle\langle\, \varphi_{\sigma,N_\sigma+1}| \\ &= (\gamma_{\text{per}})_\sigma + |\varphi_{\sigma,N_\sigma+1}\,\rangle\langle\, \varphi_{\sigma,N_\sigma+1}| - |\varphi_{\sigma,N_\sigma}\,\rangle\langle\, \varphi_{\sigma,N_\sigma}|\,, \end{aligned}$$

where $\langle \varphi_{\sigma,N_\sigma+1} \mid \varphi_{\sigma,j} \rangle = 0$ for all $j \in \{1, 2, \ldots, N_\sigma - 1\}$. Therefore, we can write

$$\widetilde{\gamma}_\xi := (\gamma_{\text{per}})_\xi + \delta_{\xi,\sigma} S,$$

where

$$S := |\varphi_{\sigma,N_\sigma+1}\,\rangle\langle\, \varphi_{\sigma,N_\sigma+1}| - |\varphi_{\sigma,N_\sigma}\,\rangle\langle\, \varphi_{\sigma,N_\sigma}|\,.$$

We compute now

$$\begin{aligned} &\mathcal{E}_{\text{hf}}(\widetilde{\gamma}) - \mathcal{E}_{\text{hf}}(\gamma_{\text{per}}) = \operatorname{Tr}\{h_\sigma\, S\} \\ &+ \frac{g}{2\,|\Gamma|^{\frac{1}{2}}} \sum_{\xi,\eta\in\Gamma^*} \int_Q \int_Q (UW)_0(x-y) \Big\{ T_\xi(x,x)\, T_\eta(y,y) - (\gamma_{\text{per}})_\xi(x,x)\, (\gamma_{\text{per}})_\eta(y,y) \Big\} dx\, dy \\ &- \frac{g}{2\,|\Gamma|^{\frac{1}{2}}} \sum_{\xi,\eta\in\Gamma^*} \int_Q \int_Q (UW)_{\xi-\eta}(x-y) \Big\{ \overline{T_\xi(x,y)}\, T_\eta(x,y) - \overline{(\gamma_{\text{per}})_\xi(x,y)}\, (\gamma_{\text{per}})_\eta(x,y) \Big\} dx\, dy, \end{aligned}$$

where $T_\xi(x,y) := (\gamma_{\rm per})_\xi(x,y) + \delta_{\xi,\sigma}\, S(x,y)$. The Kronecker-delta yields

$$\begin{aligned}
&\mathcal{E}_{\rm hf}(\widetilde{\gamma}) - \mathcal{E}_{\rm hf}(\gamma_{\rm per}) = \mathrm{Tr}\,\{h_\sigma\, S\} \\
&+ \frac{g}{|\Gamma|^{\frac{1}{2}}} \int_Q\int_Q \Big\{ (UW)_0(x-y) \Big[S(x,x) \sum_{\eta\in\Gamma^*} (\gamma_{\rm per})_\eta(y,y) + \frac{1}{2}\, S(x,x)\, S(y,y) \Big] \\
&- \mathrm{Re}\Big[\sum_{\eta\in\Gamma^*} (UW)_{\sigma-\eta}(x-y)\, \overline{S(x,y)}\, (\gamma_{\rm per})_\eta(x,y) \Big] - \frac{1}{2} (UW)_0(x-y)\, |S(x,y)|^2 \Big\} dx\, dy.
\end{aligned}$$

With (4.6) we get

$$\begin{aligned}
\mathcal{E}_{\rm hf}(\widetilde{\gamma}) - \mathcal{E}_{\rm hf}(\gamma_{\rm per}) &= \langle \varphi_{\sigma,N_\sigma+1} | H_\sigma^{(g)} \varphi_{\sigma,N_\sigma+1}\rangle - \langle \varphi_{\sigma,N_\sigma} | H_\sigma^{(g)} \varphi_{\sigma,N_\sigma}\rangle \\
&\quad + \frac{g}{2\,|\Gamma|^{\frac{1}{2}}} \int_Q\int_Q (UW)_0(x-y) \Big[S(x,x) S(y,y) - |S(x,y)|^2 \Big]
\end{aligned}$$

But if we denote $\varphi := \varphi_{\sigma,N_{\sigma+1}}$ and $\psi := \varphi_{\sigma,N_\sigma}$, then

$$\begin{aligned}
S(x,x)\, S(y,y) - |S(x,y)|^2 &= \Big(|\varphi(x)|^2 - |\psi(x)|^2 \Big) \Big(|\varphi(y)|^2 - |\psi(y)|^2 \Big) \\
&\quad - \Big| \varphi(x)\, \overline{\varphi(y)} - \psi(x)\, \overline{\psi(y)} \Big|^2 .
\end{aligned}$$

A direct computation yields

$$\begin{aligned}
S(x,x)\, S(y,y) - |S(x,y)|^2 &= -\, |\varphi(x)\, \psi(y) - \psi(x)\, \varphi(y)|^2 \\
&= -2\, |(\varphi \wedge \psi)\, (x,y)|^2
\end{aligned}$$

Therefore, we obtain

$$\begin{aligned}
e_{\sigma,N_\sigma+1} - e_{\sigma,N_\sigma} &\geq \frac{g}{|\Gamma|^{\frac{1}{2}}} \int_Q\int_Q (UW)_0(x-y)\, |(\varphi\wedge\psi)\, (x,y)|^2 \\
&= \frac{g}{|\Gamma|^{\frac{1}{2}}} \int_Q\int_Q (UW)_0(x-y)\, \Big| \Big(\varphi_{\sigma,N_{\sigma+1}} \wedge \varphi_{\sigma,N_\sigma} \Big)\, (x,y) \Big|^2 =: \Delta_{N_{\sigma+1},N_\sigma},
\end{aligned}$$

since $\gamma_{\rm per}$ is a minimizer of $\mathcal{E}_{\rm hf}$.

$\square$

Chapter 5

Opening of the Spectral Gap in the One-Dimensional Case

Contents

Summary

In the last chapter we proved that the spectral gap of the fibered effective Hamiltonian $H_\xi^{(g)}$ can be estimated by the corresponding fiber of the interaction potential parameterized by a coupling constant g. This proof does not give a rigorous numerical estimate for the gap $e_{N+1,\xi} - e_{N,\xi}$ for fixed $\xi \in \Gamma^*$. Moreover, the behavior of the spectral gap cannot be derived from this estimate if the considered system is exposed to external effects. To deal with this problem, a discrete model will be considered in 5.1 with the Hamiltonian given by the discrete Laplace operator plus an interaction. The interaction can be identified with multiplication by a symmetric positive function. Further, a decomposition of the sequence space according to a given invariance will be constructed in 5.1.1 to study the periodic properties of such

a system. This decomposition of functions into Bloch waves corresponds to a direct integral decomposition of operators K on the sequence space, in the sense that the spectral analysis of K is reduced to the analysis of the fibers of K. Applying this construction to the periodic density matrices, it will be seen in 5.1 that equivalent statements for their periodicity and an explicit formula for their fibers can be obtained. Moreover, we can prove, as we did in the continuous case (Theorem 5.1), that the eigenvectors of a Hamiltonian with periodic potential can be chosen to have the form of a plane wave multiply a function with the same periodicity. This fact is known as the Bloch theorem. We focus on the one-dimensional case, since in this case twofold degeneracy is the worst that can occur[1]. In the absence of any interaction the electronic energy levels are just a parabola in ξ as illustrated in Figure (1),

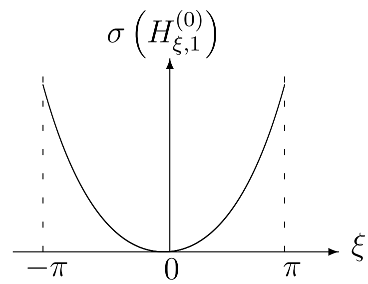

Figure (1)

where q in $H^{(0)}_{\xi,q}$, denotes the assumed periodicity. Every 1-periodic function is 2-periodic and can be considered as in Figure (2).

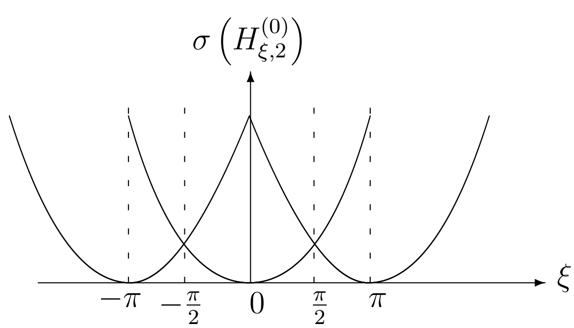

Figure (2)

In the presence of a weak one-dimensional periodic potential we have seen in Theorem 4.2 that the gap $e_{\xi,N_\xi+1} - e_{\xi,N_\xi}$ is at least $\Delta_{N_{\xi+1},N_\xi}$, which is not a negligible quantity for small systems. Moreover, this gap splits in such a way that both curves have a zero slope at $\frac{\pi}{2}$. We redraw Figure (2) to obtain Figure (3).

[1]For more details see [22]

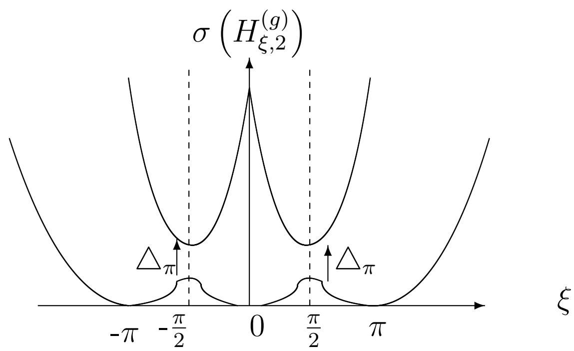

Figure (3)

When the planes and their associated intersection points are included, we end up with a set of curves such as those shown in Figure (4).

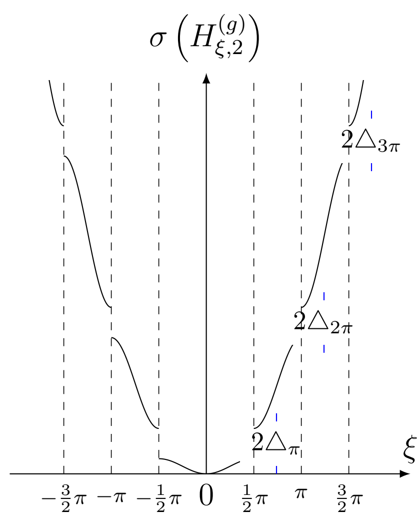

Figure (4)

If we insist on specifying all the levels by a wave vector ξ in the first Brillouin zone

$$\mathrm{BZ} := [-\pi, \pi] \cap \frac{\pi}{L}\mathbb{Z},$$

then we must translate the pieces of Figure (4) into BZ which gives Figure (5).

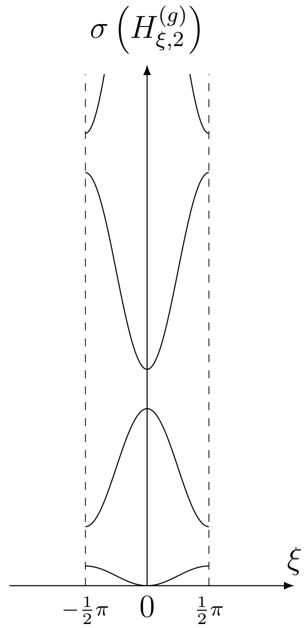

Figure (5)

Each fibered Hamiltonian is the sum of the fibered discrete Laplace operator and the fibered interaction (Lemma 5.1). The fibered discrete Laplace operator can be diagonalized directly via the above decomposition. Hence, the fibered Hamiltonian can be diagonalized owing to the symmetry of the function that defines the interaction. Its representation matrix will be computed explicitly in Lemma 5.2. Taking advantage of this representation allows us to prove in Lemma 5.3 that the distance between consecutive eigenvalues increases in the presence of a weak positive one-dimensional periodic potential.

5.1 Model and Main Result

Let $\mathfrak{H} = \ell^2(\Lambda_L)$, where $\Lambda_L = (\mathbb{Z})^d \,/\, (L\mathbb{Z})^d$ is now a finite torus with L assumed to be of the form $L = \ell q$, where $\ell, q \in \mathbb{N}$. To study the periodic properties of minimizers with periodic Γ, it is convenient to introduce the unit cell $Q = \Lambda/\Gamma = \mathbb{Z}^d/(q\mathbb{Z})^d$ and the lattice $\Gamma = (q\mathbb{Z})^d/(L\mathbb{Z})^d$. The one-particle free Hamiltonian is the operator

$$h = -\Delta^{\mathrm{disc}},$$

where the discrete Laplace operator $-\Delta^{\text{disc}}$ acting on $\varphi \in \mathfrak{H}$ is defined by

$$\left(-\Delta^{\text{disc}}\varphi\right)(x) = -\sum_{|e|=1} \{\varphi(x+e) - \varphi(x)\}, \tag{5.1}$$

Let $W : \Lambda \longrightarrow \mathbb{R}_0^+$ be a positive function, $W(x) > 0$, $\forall x \in \Lambda$ such that:

$$W(x) = W(-x), \quad \forall x \in \Lambda.$$

We identify the pair-interaction potential W acting on $\mathfrak{H} \otimes \mathfrak{H}$ with the multiplication operator by the positive and symmetric function $W(x-y)$. We are interested in showing that the distance between consecutive eigenvalues of the fibered HF Hamiltonian increases in the presence of a weak positive one-dimensional periodic potential W.

Theorem 5.1. *Let h and W be as above. For a given 1-pdm γ that satisfies*

1. $0 \leq \gamma \leq \mathbb{1}$, *with* $Tr_{\mathfrak{H}}\{\gamma\} = N$,
2. *for all $k \in \Gamma$, γ is Γ-periodic, i.e., $\tau_k\gamma = \gamma\tau_k$, where τ_k denotes the translation operator by k,*

We introduce the effective Hamiltonian $H^{(g)}(\gamma)$ defined by

$$\left[H^{(g)}(\gamma)\varphi\right](x) = (h\varphi)(x) + g\sum_{y\in\Lambda}\Big\{\gamma(y,y)\varphi(x) - \gamma(x,y)\varphi(y)\Big\}W(x-y),$$

where $\varphi \in \mathfrak{H}$ is assumed to be normalized and $0 < g \ll 1$ is a coupling constant, i.e, a positive number that determines the strength of the interaction. Then

1. *The fibered Hamiltonian is given by*

$$H_\xi^{(g)}(\gamma) = h_\xi + \frac{g}{|\Gamma|^{1/2}}\left[\sum_{\eta\in\Gamma^*}\sum_{y\in Q}(UW)_0(x-y)\gamma_\eta(y,y) - K_\xi\right],$$

   where

$$\begin{aligned}(K_\xi\varphi)(x) &= \sum_{y\in Q} K_\xi(x,y)\varphi(y) \\ &= \sum_{y\in Q}\sum_{\eta\in\Gamma^*}(UW)_{\xi-\eta}(x-y)\gamma_\eta(x,y)\varphi(y).\end{aligned}$$

2. *Let $d=1$, $\gamma_0^{per} = \mathbb{1}_N\Big[H^{(g)}(\gamma_0^{per})\Big]$ and $\{\varphi_s\}_{s\in Q}$ be the eigenfunctions of the discrete Laplace operator given in* (5.1) *corresponding to the eigenvalues $\{\lambda_s\}_{s\in Q}$. Further let $\gamma_{0,\xi}^{per}$ be the projection onto the N lowest eigenvalues of $H_\xi^{(g)}(\gamma_0^{per})$. Then the matrix representation $\widetilde{h}(g,\xi)$ of the fibered Hamiltonian $H_\xi^{(g)}(\gamma_0^{per})$ is given by*

$$\Big[\widetilde{h}(g,\xi)\Big]_{s,t} = \delta_{s,t}\lambda_{s,\xi} + \frac{2g}{q}\sum_{z\in Q}\sum_{k\in\Gamma} W(z+k)\delta_{s,t} - \frac{g}{q}\sum_{z\in Q}\sum_{r=1}^{q'} e^{\frac{-2\pi i}{q}(s-r)z}W(z)\delta_{s,t}.$$

3. *If we assume for all $|z|>R$ that $W(z)=0$ where $q\geq R$, then the difference between the s^{th} and $(s+1)^{\mathrm{st}}$ eigenvalues of $H_\xi^{(g)}$, is positive, uniformly in ℓ for $s\in\{1,\ldots,q\}$, i.e.,*

$$\liminf_{\ell\longrightarrow\infty}\left\{\left\langle\varphi_{s+1,\xi}\middle|H_\xi^{(g)}\left(\gamma_0^{per}\right)\varphi_{s+1,\xi}\right\rangle - \left\langle\varphi_{s,\xi}\middle|H_\xi^{(g)}\left(\gamma_0^{per}\right)\varphi_{s,\xi}\right\rangle\right\} > 0.$$

4. *Let $\gamma_g^{per}\in\mathscr{L}^1(\mathfrak{H})$ be a Γ-periodic, rank-N projection onto the N lowest eigenvalues of $H_\xi^{(g)}(\gamma_g^{per})$ with $0\leq\gamma_g^{\mathrm{per}}\leq 1$. Moreover, suppose that*

$$\|R_{g,\xi}\|_{HS} = \left\|\gamma_{g,\xi}^{\mathrm{per}} - \gamma_{0,\xi}^{\mathrm{per}}\right\|_{Hs} \leq cg,$$

for constant $c>0$ and W is a bounded function on Λ. Then we have

$$E_{s+1,\xi} - E_{s,\xi} \geq g.c_{\ell,\xi} > 0, \quad \inf\left\{c_{\ell,\xi} \mid \ell\in\mathbb{N}, \xi\in\Gamma^*\right\} > 0,$$

where $E_{j,\xi}$ is the j^{th} eigenvalue of $H_\xi^{(g)}(\gamma_g^{\mathrm{per}})$.

The rest of this chapter is devoted to the proof of Theorem 5.1. Before we begin the proof we repeat some definitions and remarks used in the continuous case. These will be fundamental for our proof in the discrete case.

5.1.1 Bloch Wave Decomposition

Since the periodic functions can be completely characterized by their values in the unit cell Q, the periodic problem can be reduced to Q by using the Bloch wave decomposition. Therefore, we introduce the dual lattice of Γ given by $\Gamma^* = \frac{2\pi}{L}\Lambda_\ell$ and define $\widetilde{\mathfrak{H}} := \ell^2(\Gamma^*; \ell^2(Q))$. Then there is an isometry U between $\mathfrak{H}$ and $\widetilde{\mathfrak{H}}$, the so-called Floquet operator, defined by

$$\begin{aligned} U :& \mathfrak{H} \longrightarrow \widetilde{\mathfrak{H}} \\ (U\varphi)_\xi (x) &= \frac{1}{|\Gamma|^{1/2}} \sum_{k\in\Gamma} e^{-i(k+x)\xi} \varphi(x+k), \end{aligned} \tag{5.2}$$

for all $\xi \in \Gamma^*$, $x \in Q$ and $\varphi \in \mathfrak{H}$. We remark that the operator U is unitary, since for all $\varphi, \psi \in \mathfrak{H}$ we have

$$\begin{aligned} \sum_{\xi\in\Gamma^*} \left\langle (U\varphi)_\xi \mid (U\psi)_\xi \right\rangle_{\ell^2(Q)} &= \sum_{\xi\in\Gamma^*} \sum_{x\in Q} (U\varphi)_\xi (x) \overline{(U\psi)_\xi (x)} \\ &= \sum_{\xi\in\Gamma^*} \sum_{x\in Q} \frac{1}{|\Gamma|} \sum_{k,\ell\in\Gamma} e^{i\xi(\ell-k)} \varphi(x+k) \overline{\psi(x+\ell)}. \end{aligned}$$

Using Poisson's formula we get

$$\begin{aligned} \sum_{\xi\in\Gamma^*} \left\langle (U\varphi)_\xi \mid (U\psi)_\xi \right\rangle_{\ell^2(Q)} &= \sum_{x\in Q} \sum_{k\in\Gamma} \varphi(x+k) \overline{\psi(x+k)} \\ &= \sum_{x\in\Lambda} \varphi(x) \overline{\psi(x)} \\ &= \langle \varphi \mid \psi \rangle_{\mathfrak{H}} . \end{aligned} \tag{5.3}$$

The inverse of U is U^{-1} defined for all $\xi \longrightarrow \varphi_\xi$ in $\widetilde{\mathfrak{H}}$, by

$$\left(U^{-1}\varphi\right)(x+k) = \frac{1}{|\Gamma|^{1/2}} \sum_{\xi\in\Gamma^*} e^{i(x+k)\xi} \varphi_\xi(x), \tag{5.4}$$

for all $x \in Q$. To the above decomposition of functions in $\mathfrak{H}$ into Bloch waves there corresponds a direct integral decomposition of a self-adjoint operator K on $\mathfrak{H}$ in the sense that there exists a unique bounded function

$$\begin{aligned} \Phi : \Gamma^* &\longrightarrow \mathscr{B}(\ell^2(Q)) \\ \xi &\longmapsto K_\xi, \end{aligned}$$

such that for any function $\varphi \in \mathfrak{H}$ and every $\xi \in \Gamma^*$ we have

$$(UK\varphi)_\xi = K_\xi (U\varphi)_\xi .$$

Moreover, we also have

$$\sup_{\xi\in\Gamma^*} \|K_\xi\|_{\mathscr{B}(\ell^2(Q))} = \|K\|_{\mathscr{B}(\mathfrak{H})} .$$

Definition 5.1. *1. A function $\varphi \in \mathfrak{H}$ will be called Γ-periodic if and only if*

$$\tau_k \varphi = \varphi, \forall k \in \Gamma,$$

where τ_k denotes the translation operator defined for all $\varphi \in \mathfrak{H}$ by

$$\tau_k \varphi(x) = \varphi(x+k). \tag{5.5}$$

2. An operator $\gamma \in \mathscr{L}(\mathfrak{H})$ will be called Γ-periodic if and only if

$$\tau_k \gamma = \gamma \tau_k, \forall k \in \Gamma.$$

Remark 5.1. As in the continuous case we can use the unitary operator U defined in (5.2) to get the same results on the Γ-periodicity of γ, as well as the Bloch theorem in a discrete case.

1. Let γ be a self-adjoint operator defined by its kernel $\gamma(x,y)$ for all $x, y \in \Lambda$ such that
$$\forall k \in \Gamma : \gamma(x+k, y+k) = \gamma(x,y). \tag{5.6}$$
Then the fibers of γ are given by
$$\begin{aligned} \gamma_\xi(x,y) &= e^{-i\xi(x-y)} \sum_{k\in\Gamma} e^{-ik\xi} \gamma(x+k, y) \\ &= e^{-i\xi(x-y)} \sum_{k\in\Gamma} e^{ik\xi} \gamma(x, y+k). \end{aligned} \tag{5.7}$$

2. For any sequence $(\gamma_\xi)_{\xi\in\Gamma^*}$ such that $\forall \xi \in \Gamma^*$, $\gamma_\xi \in \mathscr{L}^1(\ell^2(Q))$ satisfies
$$\gamma_\xi = \sum_{j=1}^{|Q|} \lambda_{\xi,j} \left|\varphi_{\xi,j}\right\rangle \left\langle \varphi_{\xi,j}\right|, \tag{5.8}$$
where $\lambda_{\xi,j} \in \mathbb{C}$ and $\varphi_{\xi,j} \in \ell^2(Q)$. Then the operator $\gamma = U^{-1} \bigoplus_{\xi\in\Gamma^*} \gamma_\xi U \in \mathscr{L}^1(\mathfrak{H})$ satisfies
$$\gamma = \sum_{\xi\in\Gamma^*} \sum_{j=1}^{|Q|} \lambda_{\xi,j} \left|\psi_{\xi,j}\right\rangle \left\langle \psi_{\xi,j}\right|,$$
where $\psi_{\xi,j} = \frac{1}{|\Gamma|^{\frac{1}{2}}} e^{i\xi x} \varphi_{\xi,j} \in \mathfrak{H}^\xi$.

3. Bloch's Theorem: Let $\gamma \in \mathscr{L}^1(\mathfrak{H})$ be a Γ-periodic, self-adjoint operator. Then there exists a set $(\lambda_j)_{1\leq j\leq|\Lambda|}$ in $\mathbb{R}$ and an orthonormal set of vectors $(\psi_j)_{1\leq j\leq|\Lambda|}$ in $\mathfrak{H}$ such that
$$\forall\, 1 \leq j \leq |\Lambda|\,,\ \exists \xi \in \Gamma^* \ \text{ s.t. } \ \psi_j \in \mathfrak{H}^\xi \tag{5.9}$$
and
$$\gamma = \sum_{j=1}^{|\Lambda|} \lambda_j \left|\psi_j\right\rangle \left\langle \psi_j\right| \,. \tag{5.10}$$

The proof of these results is similar to the proof in the continuous case except that we must replace integrals over Q by sums over Q.

We now show that if γ is a bounded function of a Γ-periodic, self-adjoint operator H, i.e., $\gamma = f(H)$ with a bounded measurable function f, then every fiber γ_ξ of γ can be written as $\gamma_\xi = f(H_\xi)\,, \forall \xi \in \Gamma^*$ and vice versa.

Lemma 5.1. *Let $H \in \mathscr{L}(\mathfrak{H}_\Lambda)$ be a Γ-periodic self-adjoint operator and $f : \mathbb{R} \to \mathbb{C}$ a measurable function bounded on $\sigma(H)$. Then the operator $\gamma \in \mathscr{L}(\mathfrak{H}_\Lambda)$ defined by $\gamma = f(H)$ is Γ-periodic and*

$$\forall \xi \in \Gamma^* : \quad \gamma_\xi = f\left(H_\xi\right).$$

Conversely, consider the sequence $(\gamma_\xi)_{\xi\in\Gamma^*}$ in $\mathscr{L}(\mathfrak{H}_Q)$ such that $\forall \xi \in \Gamma^*$, $\gamma_\xi = f\left(H_\xi\right)$. Then, the operator $\gamma = U^{-1}\Big(\bigoplus_{\xi\in\Gamma^*} \gamma_\xi\Big)U \in \mathscr{L}(\mathfrak{H}_\Lambda)$ satisfies $\gamma = f(H)$.

We remark that the converse in the proposition above can be written as

$$U^{-1}\Big(\bigoplus_{\xi\in\Gamma^*} f\left(H_\xi\right)\Big)U = f\Big(U^{-1}\Big(\bigoplus_{\xi\in\Gamma^*} H_\xi\Big)U\Big).$$

Proof. Since H is Γ-periodic and self-adjoint, it follows by proceeding as in the proof of Lemma 3.5 that $\forall \xi \in \Gamma^*$ there exists a set $(\lambda_{\xi,j})_{1\leq j\leq|Q|}$ in $\mathbb{R}$ and an orthonormal set of vectors $(\varphi_{\xi,j})_{1\leq j\leq|Q|}$ in $\mathfrak{H}_Q$ such that

$$H_\xi = \sum_{j=1}^{|Q|} \lambda_{\xi,j} \left|\varphi_{\xi,j}\right\rangle \left\langle \varphi_{\xi,j}\right| \,.$$

Moreover it holds that
$$H = \sum_{\xi\in\Gamma^*} \sum_{j=1}^{|Q|} \lambda_{\xi,j} \left|\psi_{\xi,j}\right\rangle \left\langle \psi_{\xi,j}\right| \,,$$

where the functions

$$\psi_{\xi,j} = \frac{1}{|\Gamma|^{\frac{1}{2}}} e^{i\xi x} \varphi_{\xi,j} \in \mathfrak{H}_\Lambda^\xi \,,$$

satisfy for all $\xi, \xi' \in \Gamma^*$ and all $1 \le j, j' \le |Q|$ the orthonormality property:

$$\langle \psi_{\xi,j}, \psi_{\xi',j'} \rangle_{\mathfrak{H}_\Lambda} = \delta_{\xi,\xi'} \delta_{j,j'} \,.$$

It then follows that

$$f(H_\xi) = \sum_{j=1}^{|Q|} f(\lambda_{\xi,j}) \, |\varphi_{\xi,j}\rangle \langle \varphi_{\xi,j}| \,, \tag{5.11}$$

and also

$$f(H) = \sum_{\xi \in \Gamma^*} \sum_{j=1}^{|Q|} f(\lambda_{\xi,j}) \, |\psi_{\xi,j}\rangle \langle \psi_{\xi,j}| \,. \tag{5.12}$$

Consider now the operator $\gamma = f(H)$. Since $\psi_{\xi,j} \in \mathfrak{H}_\Lambda^\xi$, then equation (5.12) implies that γ is Γ-periodic, and using $(U\psi_{\xi_0,j})_\xi = \delta_{\xi_0,\xi}\varphi_{\xi_0,j}$ we get for all $\psi \in \mathfrak{H}_\Lambda$ and $\xi \in \Gamma^*$ that

$$\begin{aligned}
(U\gamma\psi)_\xi &= \sum_{\xi_0 \in \Gamma^*} \sum_{j=1}^{|Q|} f(\lambda_{\xi_0,j}) \, \delta_{\xi_0,\xi} \varphi_{\xi_0,j} \, \langle \psi_{\xi_0,j}, \psi \rangle_{\mathfrak{H}_\Lambda} \\
&= \sum_{j=1}^{|Q|} f(\lambda_{\xi,j}) \, \varphi_{\xi,j} \sum_{\xi_0 \in \Gamma^*} \langle \delta_{\xi,\xi_0} \varphi_{\xi,j}, (U\psi)_{\xi_0} \rangle_{\mathfrak{H}_Q} \\
&= \sum_{j=1}^{|Q|} f(\lambda_{\xi,j}) \, \varphi_{\xi,j} \, \langle \varphi_{\xi,j}, (U\psi)_\xi \rangle_{\mathfrak{H}_Q} \,,
\end{aligned}$$

which implies $\gamma_\xi = f(H_\xi)$. Conversely, if we consider the sequence $(\gamma_\xi)_{\xi \in \Gamma^*}$ such that $\forall \xi \in \Gamma^*$, $\gamma_\xi = f(H_\xi)$, it follows from equations (5.11) and (5.12) and Lemma 3.4 that the operator

$$\gamma = U^{-1} \Big(\bigoplus_{\xi \in \Gamma^*} \gamma_\xi \Big) U,$$

satisfies $\gamma = f(H)$.

□

5.1.2 The Fibers of the Effective HF Hamiltonian

We note that the effective Hamiltonian $H^{(g)}$ can be written in the form

$$H^{(g)} = h + g(W_\gamma^1 - W_\gamma^2),$$

where W_γ^1 is multiplication by the function

$$W_\gamma^1(x) = \sum_{y\in\Lambda} W(x-y)\gamma(y,y),$$

and W_γ^2 is the operator with kernel

$$W_\gamma^2(x,y) = W(x-y)\gamma(x,y).$$

We will now show that $H^{(g)}$ is Γ-periodic if γ is Γ-periodic and give its fibers in an explicit formula.

Lemma 5.2. *Let γ be a self-adjoint operator on $\mathfrak{H}$ which satisfies* (5.6). *Then the effective Hamiltonian $H^{(g)}$ is Γ-periodic, i.e.,*

$$\forall k \in \Gamma : \tau_k H^{(g)} = H^{(g)}\tau_k,$$

where τ_k denotes the translation operator defined for all $\varphi \in \mathfrak{H}$ as in (5.5) *and its fibers are given by*

$$H_\xi^{(g)}(\gamma) = h_\xi + \frac{g}{|\Gamma|^{1/2}}\left[\sum_{\eta\in\Gamma^*}\sum_{y\in Q}(UW)_0(x-y)\gamma_\eta(y,y) - K_\xi\right],$$

for all $\xi \in \Gamma^*$, where

$$\begin{aligned}(K_\xi\varphi)(x) &= \sum_{y\in Q} K_\xi(x,y)\varphi(y)\\ &= \sum_{y\in Q}\sum_{\eta\in\Gamma^*}(UW)_{\xi-\eta}(x-y)\gamma_\eta(x,y)\varphi(y).\end{aligned}$$

Proof. Owing to (5.1) we have

$$\begin{aligned}(\tau_k h\varphi)(x) &= \left(-\Delta^{\mathrm{disc}}\varphi\right)(x+k)\\ &= -\sum_{|e|=1}\{\varphi(x+k+e)-\varphi(x+k)\}\\ &= \left(-\Delta^{\mathrm{disc}}\tau_k\varphi\right)(x)\\ &= (h\tau_k\varphi)(x).\end{aligned}$$

Moreover, we remark that

$$\begin{aligned}\left(\tau_k W_\gamma^1 \varphi\right)(x) &= \left(W_\gamma^1 \varphi\right)(x+k)\\ &= W_\gamma^1(x+k)\varphi(x+k)\\ &= \left(\sum_{y\in\Lambda}\gamma(y,y)W(x+k-y)\right)\varphi(x+k).\end{aligned}$$

Changing y to $y+k$ we get

$$\left(\tau_k W_\gamma^1 \varphi\right)(x) = \left(\sum_{y\in\Lambda}\gamma(y+k,y+k)W(x-y)\right)\varphi(x+k).$$

Using (5.6) we obtain the periodicity of the multiplication operator, i.e.,

$$\begin{aligned}\left(\tau_k W_\gamma^1 \varphi\right)(x) &= \left(\sum_{y\in\Lambda}\gamma(y,y)W(x-y)\right)\varphi(x+k)\\ &= \left(W_\gamma^1(\tau_k\varphi)\right)(x).\end{aligned}$$

Similarly we prove the periodicity of the kernel operator W_γ^2. Indeed,

$$\begin{aligned}\left(\tau_k W_\gamma^2 \varphi\right)(x) &= \left(W_\gamma^2 \varphi\right)(x+k)\\ &= \sum_{\Lambda}\gamma(x+k,y)\varphi(y)W(x+k-y).\end{aligned}$$

Again changing y to $y+k$ and using the periodicity of the kernel of γ stated in (5.6) yield

$$\begin{aligned}\left(\tau_k W_\gamma^2 \varphi\right)(x) &= \sum_{\Lambda}\gamma(x,y)\varphi(y+k)W(x-y)\\ &= \left(W_\gamma^2 \tau_k\varphi\right)(x).\end{aligned}$$

Thus, the effective Hamiltonian is Γ-periodic. Its fibers are computed as follows. For the one-particle operator $h = -\Delta^{\mathrm{disc}}$ we have

$$\left[U(-\Delta^{\mathrm{disc}})\varphi\right]_\xi(x) = -\sum_{|e|=1}\left\{(U\tau_e\varphi)_\xi(x) - (U\varphi)_\xi(x)\right\}.$$

Using the Floquet operator U gives

$$\begin{aligned}(U\tau_e\varphi)_\xi(x) &= \frac{1}{|\Gamma|^{1/2}}\sum_{k\in\Gamma} e^{-i(x+k)\xi}\varphi(x+e+k)\\ &= \frac{e^{i\xi e}}{|\Gamma|^{1/2}}\sum_{k\in\Gamma} e^{-i(x+k+e)\xi}\varphi(x+e+k)\\ &= e^{i\xi e}(U\varphi)_\xi(x+e).\end{aligned}$$

Therefore,

$$\begin{aligned}\Big(U(-\Delta^{\mathrm{disc}})U^{-1}\varphi\Big)_\xi(x) &= -\sum_{|e|=1}\Big\{e^{i\xi e}\varphi(x+e)-\varphi(x)\Big\}\\ &= -\sum_{y\in Q}\sum_{|e|=1}\Big\{e^{i\xi e}\delta_{x+e,y}-\delta_{x,y}\Big\}\varphi(y) \quad := \Big(-\Delta_\xi^{\mathrm{disc}}\varphi\Big)(x).\end{aligned}$$

Thus the fibers of the one-particle operator h is given by h_ξ where $h_\xi := -\Delta_\xi^{\mathrm{disc}}$ for all $\xi \in \Gamma^*$. Further, since the multiplication operator W_γ^1 is Γ-periodic we have

$$\Big(UW_\gamma^1U^{-1}\varphi\Big)(x) = \Big(W_\gamma^1\varphi\Big)(x),$$

which can be written as follows

$$\Big(UW_\gamma^1U^{-1}\varphi\Big)(x) = \frac{1}{|\Gamma|^{1/2}}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}(UW)_0(x-y)\gamma_\eta(y,y)\varphi(x).$$

Since we have

$$\begin{aligned}&\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}(UW)_0(x-y)\gamma_\eta(y,y)\varphi(x)\\ &= \sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\frac{1}{|\Gamma|^{1/2}}\sum_{k\in\Gamma}W(x-y+k)\gamma_\eta(y,y)\varphi(x),\end{aligned}$$

With (5.7) we obtain

$$\begin{aligned}&\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}(UW)_0(x-y)\,\gamma_\eta(y,y)\,\varphi(x)\\ &= |\Gamma|^{1/2}\sum_{x,y\in Q}\sum_{k\in\Gamma}W(x-y+k)\,\gamma(y,y)\,\varphi(x).\end{aligned}$$

Since γ satisfies (5.6) we conclude that

$$\begin{aligned}
&\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q} (UW)_0\,(x-y)\gamma_\eta(y,y)\varphi(x)\\
&= |\Gamma|^{1/2} \sum_{x,y\in\Lambda} W(x-y)\gamma(y,y)\varphi(x)\\
&= |\Gamma|^{1/2} \left(W^1_\gamma\varphi\right)(x).
\end{aligned}$$

Furthermore, the kernel of the operator W^2_γ satisfies

$$\left(W^2_\gamma\right)^*(x,y) = W^2_\gamma(y,x),$$

since γ is a self-adjoint operator and W is real and symmetric. Therefore a similar computation as in (5.7) implies

$$\left(UW^2_\gamma U^{-1}\varphi\right)_\xi(x) = \sum_{y\in Q} e^{-i\xi(x-y)}\sum_{k\in\Gamma} e^{-ik\xi} W^2_\gamma(x+k,y)\varphi(y).$$

Using the Floquet operator U we get

$$\left(UW^2_\gamma U^{-1}\varphi\right)_\xi(x) = |\Gamma|^{1/2}\sum_{y\in Q} e^{i\xi y}\left(UW^2_\gamma(.,y)\right)_\xi(x)\varphi(y).$$

But on the one hand we have

$$\begin{aligned}
\left(UW^2_\gamma U^{-1}\varphi\right)_\xi(x) &= |\Gamma|^{1/2}\sum_{y\in Q} e^{i\xi y}\left(U\gamma(.,y)W(.-y)\right)_\xi(x)\\
&= \sum_{y\in Q} e^{i\xi y}\sum_{k\in\Gamma} e^{-i(x+k)\xi}\gamma(x+k,y)W(x-y+k).
\end{aligned}$$

and on the other hand we have

$$\begin{aligned}
&\sum_{\eta\in\Gamma^*}\sum_{y\in Q} (UW)_{\xi-\eta}(x-y)\gamma_\eta(x,y)\\
&= |\Gamma|^{-1/2}\sum_{\eta\in\Gamma^*}\sum_{y\in Q}\sum_{k\in\Gamma} e^{-i(\xi-\eta)(x-y+k)} W(x-y+k)\gamma_\eta(x,y).
\end{aligned}$$

Using (5.7) again we obtain

$$\begin{aligned}
&\sum_{\eta\in\Gamma^*}\sum_{y\in Q} (UW)_{\xi-\eta}(x-y)\gamma_\eta(x,y)\\
&= |\Gamma|^{-1/2}\sum_{\eta\in\Gamma^*}\sum_{y\in Q}\sum_{k\in\Gamma} e^{-i(\xi-\eta)(x-y+k)}\,W(x-y+k)\,e^{-i\eta(x-y)}\sum_{l\in\Gamma} e^{-il\eta}\,\gamma(x+l,y)\\
&= |\Gamma|^{-1/2}\sum_{\eta\in\Gamma^*}\sum_{y\in Q}\sum_{k\in\Gamma}\sum_{l\in\Gamma} e^{-i\xi)(x-y+k)}\,W(x-y+k)\,e^{-i\eta(k-l)}\,\gamma(x+l,y).
\end{aligned}$$

Finally with Poisson's formula we deduce

$$\begin{aligned}
&\sum_{\eta\in\Gamma^*}\sum_{y\in Q}(UW)_{\xi-\eta}(x-y)\,\gamma_\eta(x,y)\\
&=|\Gamma|^{1/2}\sum_{y\in Q}\sum_{k\in\Gamma}e^{-i\xi(x-y+k)}\,\gamma(x+k,y)\,W(x-y+k)\\
&=|\Gamma|^{1/2}\left(U\,W_\gamma^2\,U^{-1}\varphi\right)_\xi(x).
\end{aligned}$$

□

5.1.3 Matrix Representation of the Fibered HF Hamiltonian $H_\xi^{(g)}(\gamma_0^{\text{per}})$

The fibered HF Hamiltonian is given by a free Hamiltonian which is the fibered discrete Laplace operator plus an interaction. To get its matrix representation let us first find all real numbers λ_ξ for which there exists a non-trivial solution $\varphi\in\ell^2(Q)$ such that

$$\Delta_\xi^{\text{disc}}\varphi+\lambda_\xi\varphi=0.$$

For this purpose the discrete Fourier transformation defined on $\ell^2(Q)$ is applied

$$-\sum_{|e|=1}\left\{e^{i\xi e}\widehat{\tau_e\varphi}(s)-\widehat{\varphi}(s)\right\}=\lambda_{s,\xi}\widehat{\varphi}(s),$$

where

$$\widehat{\varphi}(s)=\sum_{x\in Q}e^{-\frac{2\pi i}{q}(s-1)x}\varphi(x),$$

for all $s\in Q^*$ and

$$\begin{aligned}
\widehat{\tau_e\varphi}(s)&=\sum_{x\in Q}e^{-\frac{2\pi i}{q}(s-1)x}\varphi(x+e)\\
&=\sum_{x+e\in Q}e^{-\frac{2\pi i}{q}(s-1)(x+e-e)}\varphi(x+e)\\
&=e^{\frac{2\pi i}{q}(s-1)e}\widehat{\varphi}(s).
\end{aligned}$$

Thus,

$$\left[-\sum_{|e|=1}\left(e^{i\left[\xi+\frac{2\pi}{q}(s-1)\right]e}-1\right)\right]\widehat{\varphi}(s)=\lambda_{s,\xi}\widehat{\varphi}(s).$$

Moreover for $d=1$, we remark that

$$-\sum_{|e|=1}\left(e^{i\left[\xi+\frac{2\pi}{q}(s-1)\right]e}-1\right)=2-\left(e^{i\left[\xi+\frac{2\pi}{q}(s-1)\right]}+e^{-i\left[\xi+\frac{2\pi}{q}(s-1)\right]}\right)$$
$$=2-2\cos\Big[\xi+\frac{2\pi}{q}(s-1)\Big].$$

If we assume for every $y\in Q^*$ that $\widehat{\varphi}_y(s)=q^{1/2}\delta_y(s)$, then

$$\lambda_{s,\xi}=2\Big[1-\cos\Big[\xi+\frac{2\pi}{q}(s-1)\Big]\Big]. \tag{5.13}$$

Furthermore, Plancherel theorem yields

$$\begin{aligned}\langle\varphi_s \mid \varphi_{s'}\rangle_{\ell^2(Q)} &= \frac{1}{q}\,\langle\widehat{\varphi}_s \mid \widehat{\varphi}_{s'}\rangle_{\ell^2(Q)}\\ &= \frac{1}{q}\left\langle q^{1/2}\delta_s \mid q^{1/2}\delta_{s'}\right\rangle_{\ell^2(Q)}\\ &= \langle\delta_s \mid \delta_{s'}\rangle_{\ell^2(Q)}\,.\end{aligned}$$

and the inverse discrete Fourier transform gives

$$\begin{aligned}\varphi_s(x) &= \frac{1}{q}\sum_{y\in Q^*} e^{\frac{2\pi i}{q}(y-1)x}\,\widehat{\varphi}_s(y)\\ &= \frac{1}{q}\sum_{y\in Q^*} e^{\frac{2\pi i}{q}(y-1)x}\,q^{1/2}\,\delta_s(y)\\ &= \frac{1}{q^{1/2}}\,e^{\frac{2\pi i}{q}(s-1)x}.\end{aligned}$$

But since $\varphi_s\in\mathfrak{H}_Q^\xi:=\Big\{\varphi\in\ell^2(Q)\mid e^{-i\xi x}\varphi_s \text{ is } \Gamma\text{-periodic}\Big\}$ as a boundary condition we get

$$\varphi_{s,\xi}(x)=\frac{1}{q^{1/2}}\,e^{i\left[\xi+\frac{2\pi}{q}(s-1)\right]x},\ x\in Q. \tag{5.14}$$

We now give the matrix representation of the fibered Hamiltonian $H_\xi^{(g)}(\gamma_0^{\mathrm{per}})$ evaluated in a state of the form (5.14) for all $s\in Q$.

Lemma 5.3. *Let $\lambda_{s,\xi}$ and $\varphi_{s,\xi}$ be as in (5.13) and (5.14) for all $s\in Q^*$ and $\xi\in\Gamma^*$. Let moreover $\gamma_0^{\mathrm{per}}=\mathbb{1}\Big[H^{(g)}\Big(\gamma_0^{\mathrm{per}}\Big)\le e_N\Big]$, where e_N the N^{th} eigenvalue of $H^{(g)}\Big(\gamma_0^{\mathrm{per}}\Big)$.*

Then the matrix representation $\widetilde{h}(g,\xi)$ of the fibered Hamiltonian $H^{(g)}_\xi(\gamma_0^{\rm per})$ is given by

$$\Big[\widetilde{h}(g,\xi)\Big]_{s,t} = \delta_{s,t}\,\lambda_{s,\xi} + \frac{2g}{q}\sum_{z\in Q}\sum_{k\in\Gamma} W(z+k)\,\delta_{s,t}$$
$$-\frac{g}{q}\sum_{z\in Q}\sum_{r=1}^{q'} e^{\frac{2\pi i}{q}(s-r)z}\,W(z)\,\delta_{s,t}.$$

Proof. For all $s\in\{1,\dots q\}$ we have according to (5.13) and (5.14)

$$\lambda_{s,\xi} = 2\Big[1-\cos\Big(\xi+\frac{2\pi}{q}(s-1)\Big)\Big]$$
$$\varphi_s(x,\xi) = \frac{1}{q^{1/2}}e^{i\left(\xi+\frac{2\pi}{q}(s-1)\right)x}. \tag{5.15}$$

Further, owing to the Bloch's Theorem, any periodic self-adjoint operator on $\mathfrak{H}$ is given by

$$\gamma^{\rm per}_{0,\xi} = \sum_{t=1}^{q'} \mu_{t,\xi}\mid \varphi_{t,\xi}\rangle\langle\varphi_{t,\xi}\mid, \tag{5.16}$$

where $q'\in\{1,\dots,q\}$ and $\mu_{t,\xi}\in\{0,1\}$ since $\gamma^{\rm per}_{0,\xi}$ is a projection. Therefore, as in Lemma 5.2 we have

$$\Big\langle\varphi_{s,\xi}\mid H^{(g)}_\xi\varphi_{t,\xi}\Big\rangle_{\ell^2(Q)} = \langle\varphi_{s,\xi}\mid h\varphi_{t,\xi}\rangle_{\ell^2(Q)} + v_{st,\xi},$$

where

$$v_{st,\xi} = +\frac{g}{|\Gamma|^{1/2}}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\overline{\varphi_{s,\xi}(y)}(UW)_0(x-y)\gamma^{\rm per}_{0,\eta}(x,x)\varphi_{t,\xi}(y)$$
$$-\frac{g}{|\Gamma|^{1/2}}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\overline{\varphi_{s,\xi}(x)}(UW)_{\xi-\eta}(x-y)\overline{\gamma^{\rm per}_{0,\eta}(x,y)}\varphi_{t,\xi}(y).$$

Using (5.15) and (5.16) we conclude that

$$v_{st,\xi} = \frac{g}{|\Gamma|^{\frac12}}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\sum_{k\in\Gamma}\frac{1}{|\Gamma|^{\frac12}}W(x-y+k)\left(\frac{q'}{q}\right)\left(\frac1q e^{\frac{2\pi i}{q}(s-t)y}\right)$$
$$-\frac{g}{|\Gamma|^{\frac12}}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\sum_{k\in\Gamma}\frac{1}{|\Gamma|^{\frac12}}e^{-i(\xi-\eta)(x-y+k)}W(x-y+k)$$
$$\cdot\left(\frac1q\sum_{r=1}^{q'}e^{-i\left(\eta+\frac{2\pi}{q}(r-1)\right)(x-y)}\right)\left(\frac1q e^{i\left(\xi(x-y)+\frac{2\pi}{q}[(s-1)x-(t-1)y]\right)}\right),$$

which is equivalent to

$$\begin{aligned}v_{st,\xi} = &\frac{gq'}{q^2\,|\Gamma|}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\sum_{k\in\Gamma} W(x-y+k)e^{\frac{2\pi i}{q}(s-t)y}\\
&-\frac{g}{q^2\,|\Gamma|}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\sum_{k\in\Gamma} e^{-ik(\xi-\eta)}W(x-y+k)\\
&\cdot\left(\sum_{r=1}^{q'} e^{-\frac{2\pi i}{q}(r-1)(x-y)}\right)\left(e^{\frac{2\pi i}{q}[(s-1)x-(t-1)y]}\right).\end{aligned}$$

With Poisson's formula we get

$$\begin{aligned}v_{st,\xi} = &\frac{gq'}{q^2}\sum_{x,y\in Q}\sum_{k\in\Gamma} W(x-y+k)e^{\frac{2\pi i}{q}(s-t)y}\\
&-\frac{g}{q^2}\sum_{x,y\in Q} W(x-y)\left(\sum_{r=1}^{q'} e^{-\frac{2\pi i}{q}(r-1)(x-y)}\right)e^{\frac{2\pi i}{q}[(s-1)x-(t-1)y]}.\end{aligned}$$

Setting $z = x-y$ yields

$$\begin{aligned}v_{st,\xi} = &\frac{gq'}{q^2}\sum_{y,z\in Q}\sum_{k\in\Gamma} W(z+k)e^{\frac{2\pi i}{q}(s-t)y}\\
&-\frac{g}{q^2}\sum_{y,z\in Q} W(z)\left(\sum_{r=1}^{q'} e^{-\frac{2\pi i}{q}(r-1)z}\right)e^{\frac{2\pi i}{q}[(s-1)z+(s-t)y]}.\end{aligned}$$

Again using Poisson's formula we obtain

$$\begin{aligned}v_{st,\xi} = &\frac{gq'}{q}\sum_{z\in Q}\sum_{k\in\Gamma} W(z+k)\delta_{s,t}\\
&-\frac{g}{q}\sum_{z\in Q} W(z)\left(\sum_{r=1}^{q'} e^{-\frac{2\pi i}{q}z(s-r)}\right)\delta_{s,t}.\end{aligned}\tag{5.17}$$

Thus,

$$\begin{aligned}\left[\widetilde{h}(g,\xi)\right]_{s,t} = &\delta_{st}\lambda_{s,\xi} + \frac{q'g}{q}\sum_{z\in Q}\sum_{k\in\Gamma} W(z+k)\delta_{s,t}\\
&-\frac{g}{q}\sum_{z\in Q} W(z)\left(\sum_{r=1}^{q'} e^{-\frac{2\pi i}{q}z(s-r)}\right)\delta_{s,t}.\end{aligned}$$

□

Remark 5.2. • Owing to the symmetry of the function $W(x)$ for all $x \in \Lambda$ the last result can be written as

$$\left\langle \varphi_{s,\xi} \mid H_\xi^{(g)} \varphi_{t,\xi} \right\rangle_{\ell^2(Q)} = \delta_{s,t}\, \lambda_{s,\xi} + \frac{2g}{q} \sum_{z\in Q} \sum_{k\in\Gamma} W(z+k)\, \delta_{s,t} - \frac{g}{q} \sum_{z\in Q} \sum_{r=1}^{q'} \cos\left(\frac{2\pi}{q}(s-r)z\right) W(z)\, \delta_{s,t}. \tag{5.18}$$

Indeed, this can be shown as follows

$$\sum_{z\in Q}\sum_{r=1}^{q'} e^{\frac{-2\pi i}{q}(s-r)z} W(z) = \frac{1}{2}\sum_{z\in Q}\sum_{r=1}^{q'} e^{\frac{-2\pi i}{q}(s-r)z} W(z) + \frac{1}{2}\sum_{z\in Q}\sum_{r=1}^{q'} e^{\frac{2\pi i}{q}(s-r)z}\, W(-z).$$

Since $W(z)$ is symmetric we get

$$\sum_{z\in Q}\sum_{r=1}^{q'} e^{\frac{-2\pi i}{q}(s-r)z}\, W(z) = \sum_{z\in Q}\sum_{r=1}^{q'} \left(\frac{e^{\frac{2\pi i}{q}(s-r)z} + e^{\frac{-2\pi i}{q}(s-r)z}}{2} \right) W(z) = \sum_{z\in Q}\sum_{r=1}^{q'} \cos\left(\frac{2\pi}{q}(s-r)z\right) W(z). \tag{5.19}$$

• The second and the third term of equation (5.18) do not depend on ξ. Therefore, if the electrons are in the same state but in different fibers, then

$$\left\langle \varphi_{s,\xi} \mid H_\xi^{(g)} \varphi_{s,\xi} \right\rangle - \left\langle \varphi_{s,\eta} \mid H_\eta^{(g)} \varphi_{s,\eta} \right\rangle = \lambda_{s,\xi} - \lambda_{s,\eta}.$$

5.1.4 Opening Gap in the Spectrum of $H_\xi^{(g)}(\gamma_0^{\mathrm{per}})$ in the Presence of a Weak Positive One-Dimensional Periodic Potential W

We now show that a gap opens between the s^{th} and $(s+1)^{\mathrm{st}}$ eigenvalues of the fibered effective Hamiltonian $H_\xi^{(g)}$ when we add an interaction, i.e., the difference between consecutive eigenvalues lying in different states but in the same fiber is positive, uniformly in ℓ (the length of the lattice Γ), in the presence of a weak positive one-dimensional potential as stated in the following lemma:

Lemma 5.4. *Let $\lambda_{s,\xi}$ and $\varphi_{s,\xi}$ be as in (5.13) and (5.14). Let moreover $\gamma_0^{\mathrm{per}} = \mathbb{1}\Big[H^{(g)}\Big(\gamma_0^{\mathrm{per}}\Big) \leq e_N\Big]$, where e_N the N^{th} eigenvalue of $H^{(g)}\Big(\gamma_0^{\mathrm{per}}\Big)$. If we assume for all $|z| > R$ that $W(z) = 0$ where $q \geq R$, then*

$$\liminf_{\ell\longrightarrow\infty}\left\{\left\langle \varphi_{s+1,\xi}\middle| H_\xi^{(g)}\left(\gamma_0^{\mathrm{per}}\right)\varphi_{s+1,\xi}\right\rangle - \left\langle \varphi_{s,\xi}\middle| H_\xi^{(g)}\left(\gamma_0^{\mathrm{per}}\right)\varphi_{s,\xi}\right\rangle\right\} > 0.$$

Proof. Using (5.18) we get

$$\begin{aligned}\left\langle \varphi_{s+1,\xi}\middle| H_\xi^{(g)}\varphi_{s+1,\xi}\right\rangle_{\ell^2(Q)} &= \lambda_{s+1,\xi} + \frac{2g}{q}\sum_{z\in\Lambda}W(z)\\ &- \quad \frac{g}{q}\sum_{z\in Q}\sum_{r=1}^{q'}\cos\left(\frac{2\pi}{q}(s+1-r)z\right)W(z)\end{aligned}$$

and also

$$\begin{aligned}\left\langle \varphi_{s,\xi}\middle| H_\xi^{(g)}\varphi_{s,\xi}\right\rangle_{\ell^2(Q)} &= \lambda_{s,\xi} + \frac{2g}{q}\sum_{z\in\Lambda}W(z)\\ &- \frac{g}{q}\sum_{z\in Q}\sum_{r=1}^{q'}\cos\left(\frac{2\pi}{q}(s-r)z\right)W(z).\end{aligned}$$

Thus,

$$\begin{aligned}&\left\langle \varphi_{s+1,\xi}\middle| H_\xi^{(g)}\varphi_{N+1,\xi}\right\rangle_{\ell^2(Q)} - \left\langle \varphi_{s,\xi}\middle| H_\xi^{(g)}\varphi_{s,\xi}\right\rangle_{\ell^2(Q)}\\ &= \lambda_{s+1,\xi} - \lambda_{s,\xi} - \frac{g}{q}\sum_{z\in Q}\sum_{r=1}^{q'}\left\{\cos\left(\frac{2\pi}{q}(s+1-r)z\right) - \cos\left(\frac{2\pi}{q}(s-r)z\right)\right\}W(z).\end{aligned}$$

Using (5.15) and the trigonometric identities we get

$$\begin{aligned}\lambda_{s+1,\xi} - \lambda_{s,\xi} &= -2\left\{\cos\left(\xi + \frac{2\pi}{q}s\right) - \cos\left(\xi + \frac{2\pi}{q}(s-1)\right)\right\}\\ &= 4\sin\left(\xi + \frac{2\pi}{q}s - \frac{\pi}{q}\right)\sin\left(\frac{\pi}{q}\right).\end{aligned}$$

Similarly we have

$$\begin{aligned}&\cos\left(\frac{2\pi}{q}(s+1-r)z\right) - \cos\left(\frac{2\pi}{q}(s-r)z\right)\\ &= -2\sin\left(\frac{2\pi}{q}(s-r+\frac{1}{2})z\right)\sin\left(\frac{\pi}{q}z\right).\end{aligned}$$

Thus,

$$\begin{aligned}
&\left\langle \varphi_{s+1,\xi} \middle| H_\xi^{(g)} \varphi_{s+1,\xi} \right\rangle_{\ell^2(Q)} - \left\langle \varphi_{s,\xi} \middle| H_\xi^{(g)} \varphi_{s,\xi} \right\rangle_{\ell^2(Q)} \\
&= 4 \sin\left(\xi + \frac{2\pi}{q} s - \frac{\pi}{q}\right) \sin\left(\frac{\pi}{q}\right) \\
&\quad + \frac{2g}{q} \sum_{z\in Q} \sum_{r=1}^{q'} \sin\left(\frac{2\pi}{q}(s - r + \frac{1}{2})z\right) \sin\left(\frac{\pi}{q} z\right) W(z). \qquad (5.20)
\end{aligned}$$

Since $s \in \{1, \ldots, q\}$, $r \in \{1, \ldots, q'\}$ with $q' \leq q$ and W is non-negative, where $W(z) = 0$ for all $|z| \geq R$ and $q \geq R$ we have

$$\left| \frac{2\pi}{q}(s - r + \frac{1}{2})z \right| \leq \frac{2\pi}{q}\Big(q - \frac{1}{2}\Big) R \leq \frac{\pi}{4},$$

for

$$R \leq \frac{q}{8q - 4}.$$

Thus, $\sin\left(\frac{2\pi}{q}(s - r + \frac{1}{2})z\right)$ and $\sin\left(\frac{\pi}{q}z\right)$ have the same sign and therefore the difference (5.20) is positive, uniformally in ℓ. □

Remark 5.3. In the case of the Hubbard model the computed gap is given by

$$\Delta_{s+1,s}(\xi, g, q, q') = \frac{2g}{q} \sum_{z\in Q} \sum_{r=1}^{q'} \sin\Big(\frac{2\pi}{q}\Big(s - r + \frac{1}{2}\Big)z\Big) \sin\Big(\frac{\pi}{q} z\Big) \delta_{z,0} = 0,$$

for $s \in \{1, \ldots, q\}$ and $q' < q$. But we know for $q = 2$, $q' = 1$, that the energy gap for the Hubbard model can be calculated exactly from the Lieb and Wu solution ([20], see also [32]) and one finds for small g that

$$\Delta_{s+1,s}(\xi, g, q, q') \sim e^{-c/g}.$$

This shows the singularity of the Hubbard model in one-dimension and assures the importance of having an interaction with non-zero range to obtain such a gap.

Now the question arises weather we can prove the last lemma for $\gamma_g^{\mathrm{per}} \in \mathscr{L}^1(\mathfrak{H})$, which is a Γ-periodic, a rank-N-projection and a self-adjoint operator on $\mathfrak{H}$. The following lemma answers that affirmatively:

Lemma 5.5. *Let $\gamma_g^{\text{per}} \in \mathscr{L}^1(\mathfrak{H})$ be a Γ-periodic, a rank-N projection and a self-adjoint operator on $\mathfrak{H}$. Moreover, suppose that*

$$\|R_{g,\xi}\|_{HS} = \left\|\gamma_{g,\xi}^{\text{per}} - \gamma_{0,\xi}^{\text{per}}\right\|_{HS} \leq cg,$$

for some constant $c > 0$ and W is a bounded function on Λ. Then

$$E_{s+1,\xi} - E_{s,\xi} \geq g.c_{\ell,\xi} > 0, \quad \inf\{c_{\ell,\xi} \mid \ell \in \mathbb{N}, \xi \in \Gamma^*\} > 0,$$

where $E_{j,\xi}$ is the j^{th} eigenvalue of $H_\xi^{(g)}(\gamma_g^{\text{per}})$.

Proof. For fixed g, ξ we define

$$h(g,\xi) = h_\xi + g\mathcal{W}_\xi,$$

whose matrix representations are given by

$$\begin{aligned}
h_{st}(g,\xi) &= \left[H_\xi^{(g)}\left(\gamma_g^{\text{per}}\right)\right]_{s,t},\\
h_{st,\xi} &= \delta_{st}\lambda_{s,\xi},\\
\mathcal{W}_{st,\xi} &:= \mathcal{W}_\xi\left(\gamma_g^{\text{per}}, |\,\varphi_{t,\xi}\,\rangle\langle\,\varphi_{s,\xi}\,|\right)\\
&= \mathcal{W}_\xi\left(\gamma_0^{\text{per}}, |\,\varphi_{t,\xi}\,\rangle\langle\,\varphi_{s,\xi}\,|\right) + \mathcal{W}_\xi\left(R_g := \gamma_g^{\text{per}} - \gamma_0^{\text{per}}, |\,\varphi_{t,\xi}\,\rangle\langle\,\varphi_{s,\xi}\,|\right)\\
&=: \ v_{st,\xi} + r_{st,\xi}
\end{aligned}$$

with

$$\begin{aligned}
v_{st,\xi} = &\frac{1}{|\Gamma|^{\frac{1}{2}}}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}(UW)_0(x-y)\gamma_{0,\eta}(x,x)\overline{\varphi_{s,\xi}(y)}\varphi_{t,\xi}(y)\\
&- \frac{1}{|\Gamma|^{\frac{1}{2}}}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}(UW)_{\xi-\eta}(x-y)\overline{\gamma_{0,\eta}(x,y)\varphi_{s,\xi}(y)}\varphi_{t,\xi}(x).
\end{aligned}$$

and also

$$\begin{aligned}
r_{st,\xi} = &\frac{1}{|\Gamma|^{\frac{1}{2}}}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}(UW)_0(x-y)R_{g,\eta}(x,x)\varphi_{t,\xi}(y)\overline{\varphi_{s,\xi}(y)}\\
&- \frac{1}{|\Gamma|^{\frac{1}{2}}}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}(UW)_{\xi-\eta}(x-y)\overline{R_{g,\eta}(x,y)}\varphi_{t,\xi}(x)\overline{\varphi_{s,\xi}(y)}.
\end{aligned}$$

Using the definition (5.2) of the Floquet operator U we get

$$
\begin{aligned}
r_{st,\xi} &= \frac{1}{q\,|\Gamma|}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\sum_{k\in\Gamma} W(x-y+k)\, R_{g,\eta}(x,x)\, e^{\frac{2\pi i}{q}(t-s)y} \\
&- \frac{1}{q\,|\Gamma|}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\sum_{k\in\Gamma} e^{-i(\xi-\eta)(x-y+k)}\, W(x-y+k)\, \overline{R_{g,\eta}(x,y)}\, e^{\frac{2\pi i}{q}[(s-1)x-(t-1)y]}.
\end{aligned}
$$

Since the result is achieved for $H_\xi^{(g)}(\gamma_0^{\mathrm{per}})$ represented by the matrix $\widetilde{h}_{st}\,(g,\xi)$, i.e., the difference between consecutive eigenvalues of $H_\xi^{(g)}(\gamma_0^{\mathrm{per}})$ is positive, uniformly in ℓ according to Lemma 5.4, therefore we get our claim if we can show

$$
\langle \psi \mid \mathcal{W}_\xi(R_g)\psi\rangle \le C\cdot g\cdot q,
$$

for all normalized $\psi\in\mathbb{C}^q$. We have

$$
\langle \psi \mid \mathcal{W}_\xi(R_g)\psi\rangle = \sum_{s,t\in Q^*} \overline{\psi_s}\, r_{st,\xi}\,\psi_t.
$$

Hence, it suffices to show

$$
|r_{st,\xi}| \le C\cdot g\cdot q.
$$

for suitable constant $0<C<\infty$. We note

$$
\begin{aligned}
|r_{st,\xi}| &\le \frac{1}{q\,|\Gamma|}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\sum_{k\in\Gamma} W(x-y+k)\ |R_{g,\eta}(x,x)| \\
&\quad + \frac{1}{q\,|\Gamma|}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\sum_{k\in\Gamma} W(x-y+k)\ |R_{g,\eta}(x,y)| \\
&= \frac{1}{q\,|\Gamma|}\sum_{\eta\in\Gamma^*}\sum_{x,y\in Q}\sum_{k\in\Gamma} W(x-y+k)\Big[|R_{g,\eta}(x,x)| + |R_{g,\eta}(x,y)|\Big].
\end{aligned}
$$

Since W is a bounded function on Λ we can write

$$
|r_{st,\xi}| \le \sup_{z\in\Lambda}\Big\{W(z)\Big\}\sum_{\eta\in\Gamma^*}\left[\sum_{x\in Q}|R_{g,\eta}(x,x)| + \frac{1}{q}\sum_{x,y\in Q}|R_{g,\eta}(x,y)|\right]. \tag{5.21}
$$

But for $x\in Q$ we have $\gamma(x,x) = \sum_{y\in Q}\left|\gamma^{\frac12}(x,y)\right|^2$, and therefore

$$
\begin{aligned}
\sum_{x\in Q}|R_{g,\eta}(x,x)| &\le \sum_{x\in Q}\left|\sum_{y\in Q}\left|\left(\gamma_{g,\eta}^{\mathrm{per}}\right)^{\frac12}(x,y)\right|^2 - \sum_{y\in Q}\left|\left(\gamma_{0,\eta}^{\mathrm{per}}\right)^{\frac12}(x,y)\right|^2\right| \\
&= \sum_{x\in Q}\left|\sum_{y\in Q}\mathrm{Re}\left(\overline{\left(\gamma_{g,\eta}^{\mathrm{per}}\right)^{\frac12}}(x,y) + \overline{\left(\gamma_{0,\eta}^{\mathrm{per}}\right)^{\frac12}}(x,y)\right)\left(\left(\gamma_{g,\eta}^{\mathrm{per}}\right)^{\frac12}(x,y) - \left(\gamma_{0,\eta}^{\mathrm{per}}\right)^{\frac12}(x,y)\right)\right|.
\end{aligned}
$$

Applying the Cauchy-Schwarz Inequality with respect to y gives

$$\sum_{x\in Q}|R_{g,\eta}(x,x)| \leq \sum_{x\in Q}\left(\sum_{y\in Q}\left(\overline{(\gamma^{\mathrm{per}}_{g,\eta})^{\frac{1}{2}}}(x,y)+\overline{\left(\gamma^{\mathrm{per}}_{0,\eta}\right)^{\frac{1}{2}}}(x,y)\right)^2\right)^{\frac{1}{2}}$$
$$\cdot\left(\sum_{y\in Q}\left(\left(\gamma^{\mathrm{per}}_{g,\eta}\right)^{\frac{1}{2}}(x,y)-\left(\gamma^{\mathrm{per}}_{0,\eta}\right)^{\frac{1}{2}}(x,y)\right)^2\right)^{\frac{1}{2}}.$$

Again using Cauchy-Schwarz Inequality with respect to x yields

$$\begin{aligned}\sum_{x\in Q}|R_{g,\eta}(x,x)| &\leq \left(\sum_{x,y\in Q}\left(\overline{(\gamma^{\mathrm{per}}_{g,\eta})^{\frac{1}{2}}}(x,y)+\overline{\left(\gamma^{\mathrm{per}}_{0,\eta}\right)^{\frac{1}{2}}}(x,y)\right)^2\right)^{\frac{1}{2}}\\ &\quad\cdot\left(\sum_{x,y\in Q}\left(\left(\gamma^{\mathrm{per}}_{g,\eta}\right)^{\frac{1}{2}}(x,y)-\left(\gamma^{\mathrm{per}}_{0,\eta}\right)^{\frac{1}{2}}(x,y)\right)^2\right)^{\frac{1}{2}}\\ &\leq \left\|\left(\overline{\gamma^{\mathrm{per}}_{g,\eta}}\right)^{\frac{1}{2}}+\left(\overline{\gamma^{\mathrm{per}}_{0,\eta}}\right)^{\frac{1}{2}}\right\|_{HS}\left\|\left(\gamma^{\mathrm{per}}_{g,\eta}\right)^{\frac{1}{2}}-\left(\gamma^{\mathrm{per}}_{0,\eta}\right)^{\frac{1}{2}}\right\|_{HS}.\end{aligned}$$

Since $\gamma^{\mathrm{per}}_{g,\eta}$ and $\gamma^{\mathrm{per}}_{0,\eta}$ are projections we conclude that

$$\sum_{x\in Q}|R_{g,\eta}(x,x)| \leq \left\|\overline{\gamma^{\mathrm{per}}_{g,\eta}}+\overline{\gamma^{\mathrm{per}}_{0,\eta}}\right\|_{HS}\left\|\gamma^{\mathrm{per}}_{g,\eta}-\gamma^{\mathrm{per}}_{0,\eta}\right\|_{HS}.$$

Also, substituting this in (5.21) we get

$$\begin{aligned}&|r_{st,\xi}|\\ &\leq \sup_{z\in\Lambda}\{W(z)\}\sum_{\eta\in\Gamma^*}\left[\left\|\overline{\gamma^{\mathrm{per}}_{g,\eta}}+\overline{\gamma^{\mathrm{per}}_{0,\eta}}\right\|_{HS}\left\|\gamma^{\mathrm{per}}_{g,\eta}-\gamma^{\mathrm{per}}_{0,\eta}\right\|_{HS}+\frac{1}{q}\sum_{x,y\in Q}\left|\overline{R_{g,\eta}(x,y)}\right|\right]\\ &\leq \sup_{z\in\Lambda}\{W(z)\}\sum_{\eta\in\Gamma^*}\left[\left\|\overline{\gamma^{\mathrm{per}}_{g,\eta}}+\overline{\gamma^{\mathrm{per}}_{0,\eta}}\right\|_{HS}\left\|\gamma^{\mathrm{per}}_{g,\eta}-\gamma^{\mathrm{per}}_{0,\eta}\right\|_{HS}+\frac{1}{q}\sum_{x,y\in Q}\left|\overline{R_{g,\eta}(x,y)}\right|^2\right]\\ &= \sup_{z\in\Lambda}\{W(z)\}\sum_{\eta\in\Gamma^*}\left\|\gamma^{\mathrm{per}}_{g,\eta}-\gamma^{\mathrm{per}}_{0,\eta}\right\|_{HS}\left[\left\|\overline{\gamma^{\mathrm{per}}_{g,\eta}}+\overline{\gamma^{\mathrm{per}}_{0,\eta}}\right\|_{HS}+\frac{1}{q}\left\|\gamma^{\mathrm{per}}_{g,\eta}-\gamma^{\mathrm{per}}_{0,\eta}\right\|_{HS}\right].\end{aligned}$$

By assumption $\left\|\gamma^{\mathrm{per}}_{g,\eta}-\gamma^{\mathrm{per}}_{0,\eta}\right\|_{HS}\leq cg$ for $c>0$, thus

$$|r_{st,\xi}| \leq cg\,\|W\|_\infty\sum_{\eta\in\Gamma^*}\left[\left\|\overline{\gamma^{\mathrm{per}}_{g,\eta}}+\overline{\gamma^{\mathrm{per}}_{0,\eta}}\right\|_{HS}+\frac{cg}{q}\right].$$

$\square$

Appendices

Appendix A

The Expression of the Hartree-Fock Functional in Terms of Density Matrices

Density matrices are used in quantum mechanics to describe a quantum system in which certain details are omitted. In fact they contain information about the status of the ensemble of spins at a given time, and therefore, their formalism can be used to represent the quantum states in a simpler way. Moreover, they can be used to generate probability distributions in different bases, as well as averages of different observables. To make contact with our analysis approach we replace the density matrices with algebraic operators, which make it easier to specify solutions for the eigenstate and eigenvalue equations for the system as well as to determine the probability of obtaining a predicted value in a measurement of the system. To describe density matrices, we consider the fermion Fock space $\mathcal{F}(\mathfrak{H})$ over a one-particle Hilbert space $\mathfrak{H}$

$$\mathcal{F}(\mathfrak{H}) = \bigoplus_{N=0}^{\infty} \mathcal{F}^{(N)}(\mathfrak{H}) \quad \text{and} \quad \mathcal{F}^{(N)}(\mathfrak{H}) := \bigwedge^{N} \mathfrak{H},$$

where $\mathcal{F}^{(0)}(\mathfrak{H}) := \mathbb{C}\Omega$ is the vacuum vector, and Ω the normalized vacuum vector. It is convenient to represent the fermion Fock space $\mathcal{F}(\mathfrak{H})$ in terms of creation and annihilation operators, $c^*(f)$ and $c(g)$, defined by

$$\begin{aligned} c^*(f)\left[c^*(\varphi_2)\ldots c^*(\varphi_N)\Omega\right] &:= c^*(f)c^*(\varphi_2)\ldots c^*(\varphi_N)\Omega \\ &:= f \wedge \varphi_2 \wedge \ldots \wedge \varphi_N \\ c(g) &:= \left(c^*(g)\right)^*, \end{aligned}$$

for all $f, g, \varphi_1, \varphi_2, \dots, \varphi_N \in \mathfrak{H}$, where

$$\varphi_1 \wedge \varphi_2 \wedge \dots \wedge \varphi_N := (N!)^{-1/2} \sum_{\pi \in S_N} (-1)^\pi \, \varphi_{\pi(1)} \otimes \varphi_{\pi(2)} \otimes \dots \otimes \varphi_{\pi(N)}.$$

Hence we can write

$$\mathcal{F}^{(N)}(\mathfrak{H}) = \overline{\operatorname{Span}\{c^*(\varphi_1) \dots c^*(\varphi_N)\Omega \mid \varphi_1, \varphi_2, \dots, \varphi_N \in \mathfrak{H}\}},$$

i.e., $\mathcal{F}(\mathfrak{H})$ is the norm closure of polynomials in creation operators acting on the vacuum vector. Moreover, the annihilation operators and their adjoint satisfy the canonical anti-commutation relations (CAR):

$$\begin{aligned} \forall \varphi, \psi \in \eta: \ & \{c(\varphi), c(\psi)\} = \{c^*(\varphi), c^*(\psi)\} = 0 \\ & \{c(\varphi), c^*(\psi)\} = \langle \varphi | \psi \rangle \\ & c(\varphi)\Omega = 0, \end{aligned} \tag{A.1}$$

where the anti-commutator $\{.,.\}$ is defined as $\{A, B\} := AB + BA$. Note that the fermion creation and annihilation operators are bounded

$$\|c^*(f)\|_{op} = \|c(f)\|_{op} = \|f\|_{\mathfrak{H}},$$

since for all $\Psi \in \mathcal{F}(\mathfrak{H})$ thanks to (A.1) we have

$$\begin{aligned} \|c^*(f)\Psi\|^2_{\mathcal{F}(\mathfrak{H})} + \|c(f)\Psi\|^2_{\mathcal{F}(\mathfrak{H})} &= \langle \Psi | \{c(f), c^*(f)\} \Psi \rangle \\ &= \|f\|^2_{\mathfrak{H}} \cdot \|\Psi\|^2_{\mathcal{F}(\mathfrak{H})}. \end{aligned}$$

Therefore $c^*(f)$ and $c(f)$ are bounded operators for all $f \in \mathfrak{H}$. Further, we get

$$\|c^*(f)\|_{op}, \|c(f)\|_{op} \leq \|f\|_{\mathfrak{H}}.$$

On the other hand we have

$$\begin{aligned} \|c^*(f)\Omega\|_{\mathcal{F}(\mathfrak{H})} &= \|f\|_{\mathfrak{H}} = \|f\|_{\mathfrak{H}} \|\Omega\|_{\mathcal{F}(\mathfrak{H})} \\ \|c(f)(c^*(f)\Omega)\|_{\mathcal{F}(\mathfrak{H})} &= \|\{c(f), c^*(f)\}\Omega\|_{\mathcal{F}(\mathfrak{H})} \\ &= \|\langle f|f\rangle_{\mathfrak{H}}\Omega\|_{\mathcal{F}(\mathfrak{H})} = \|f\|^2_{\mathfrak{H}} = \|f\|_{\mathfrak{H}} \|c^*(f)\Omega\|_{\mathcal{F}(\mathfrak{H})}. \end{aligned}$$

We also obtain that

$$\|c^*(f)\|_{op}, \|c(f)\|_{op} \geq \|f\|_{\mathfrak{H}}.$$

Definition A.1. *Let $\mathfrak{H}$ be a Hilbert space.*

1. *A density matrix is a positive operator $\rho \in \mathscr{B}(\mathcal{F}(\mathfrak{H}))$ of unit trace, i.e.,*

$$0 \leq \rho \leq \mathrm{Tr}_{\mathcal{F}} \{\rho\} = 1.$$

2. *If $\rho \in \mathscr{B}(\mathcal{F}(\mathfrak{H}))$ is a density matrix, we define its one-particle density matrix (1-pdm) $\gamma_\rho^{(1)}$ to be the bounded linear operator*

$$\gamma_\rho^{(1)} : \mathfrak{H} \longrightarrow \mathfrak{H}$$

determined by

$$\langle f | \gamma_\rho^{(1)} g \rangle_{\mathfrak{H}} := \mathrm{Tr}_{\mathcal{F}} \{\rho c^*(g) c(f)\},$$

for all $f, g \in \mathfrak{H}$.

3. *If $\rho \in \mathscr{B}(\mathcal{F}(\mathfrak{H}))$ is a density matrix, we define its two-particle density matrix (2-pdm) $\gamma_\rho^{(2)}$ to be the bounded linear operator*

$$\gamma_\rho^{(2)} : \mathfrak{H} \otimes \mathfrak{H} \longrightarrow \mathfrak{H} \otimes \mathfrak{H}$$

determined by

$$\langle f \otimes f' | \gamma_\rho^{(1)} (g \otimes g') \rangle_{\mathfrak{H} \times \mathfrak{H}} := \mathrm{Tr}_{\mathcal{F}} \{\rho c^*(g') c^*(g) c(f') c(f)\}.$$

for all $f, f', g, g' \in \mathfrak{H}$.

Lemma A.1. *Let $\rho \in \mathscr{B}(\mathcal{F}(\mathfrak{H}))$ be a density matrix and*

$$\mathcal{N} := \sum_{i=1}^{\infty} c_i^* \, c_i = \bigoplus_{N=0}^{\infty} N \cdot \mathbb{1}_{\mathcal{F}^{(N)}(\mathfrak{H})}$$

the number operator on $\mathcal{F}(\mathfrak{H})$. Suppose $\mathrm{Tr}_{\mathcal{F}(\mathfrak{H})} \{\rho \mathcal{N}^2\} < \infty$. Then the following statements are true

1. *The 1-pdm $\gamma_\rho^{(1)}$ and the 2-pdm $\gamma_\rho^{(2)}$ are bounded operators on $\mathfrak{H}$ and $\mathfrak{H} \otimes \mathfrak{H}$ respectively.*

2. *The 1-pdm $\gamma_\rho^{(1)}$ satisfies $0 \leq \gamma_\rho^{(1)} \leq \mathbb{1}$, $\mathrm{Tr}_{\mathfrak{H}} \left\{\gamma_\rho^{(1)}\right\} = \mathrm{Tr}_{\mathcal{F}} \{\rho \mathcal{N}\}$.*

3. *The 1-pdm $\gamma_\rho^{(1)}$ is an orthogonal projection of rank N onto a set of orthonormal orbitals $\varphi_1, \ldots, \varphi_N \in \mathfrak{H}$, if and only if ρ is a projection of rank 1 onto a Slater determinant $\phi = \varphi_1 \wedge \varphi_2 \cdots \wedge \varphi_N$, i.e.,*

$$\begin{aligned} \gamma_\rho^{(1)} &= \sum_{n=1}^{N} |\varphi_n\rangle\langle\varphi_n| = \left(\gamma_\rho^{(1)}\right)^2 \\ &\Longleftrightarrow \{\rho = |\phi\rangle\langle\phi|, \phi = \varphi_1 \wedge \varphi_2 \ldots \wedge \varphi_N\}\,. \end{aligned} \tag{A.2}$$

4. *The 2-pdm $\gamma_\rho^{(2)}$ satisfies $0 \le \gamma_\rho^{(2)} \le \mathrm{Tr}_{\mathcal{F}}\{\rho\mathbb{N}\}\cdot\mathbb{1}$, $Tr_{\mathfrak{H}}\left\{\gamma_\rho^{(2)}\right\} = \mathrm{Tr}_{\mathcal{F}}\{\rho\mathcal{N}(\mathcal{N}-1)\}$.*

Examples and remarks:

- In general $\gamma_\rho^{(1)} - \left(\gamma_\rho^{(1)}\right)^2 \ge 0$.
- If $\gamma_\rho^{(1)}$ is a projection of rank N, then $\gamma_\rho^{(2)}$ is a projection of rank $N(N-1)$ and we have

$$\begin{aligned} \gamma_\rho^{(2)} &= \sum_{n,m=1}^{N} |\varphi_n \wedge \varphi_m\rangle\langle\varphi_n \wedge \varphi_m| \\ &= \sum_{n,m=1}^{N} \frac{1}{2}\,|\varphi_n \otimes \varphi_m - \varphi_m \otimes \varphi_n\rangle\langle\varphi_n \otimes \varphi_m - \varphi_m \otimes \varphi_n| \\ &= \gamma_\rho^{(1)} \otimes \gamma_\rho^{(1)} - \mathrm{Ex}\left(\gamma_\rho^{(1)} \otimes \gamma_\rho^{(1)}\right) \end{aligned}$$

  where $\mathrm{Ex}\,(f \otimes g) = g \otimes f$ is the exchange operator.

Definition A.2. *Let h be a self-adjoint, semibounded operator, $h \ge -C+1$ for some constant C, on the one-particle Hilbert space $\mathfrak{H}$ and V be a symmetric, a positive operator on the Hilbert space $\mathfrak{H} \times \mathfrak{H}$ which commutes with the exchange operator, i.e. $[V, \mathrm{Ex}] = 0$, and obeying:*

$$0 \le V \le \frac{1}{4}(h \otimes 1 + 1 \otimes h) + c.$$

Moreover, let

$$H = \sum_{i,j=1}^{\infty} h_{i,j} c_i^* c_j + \sum_{i,j,k,m=1}^{\infty} V_{i,j,k,m} c_j^* c_i^* c_k c_m$$

be the Hamilton operator on $\mathfrak{H}$ where

$$\begin{aligned} h_{i,j} &:= \langle\varphi_i | h\varphi_j\rangle \\ V_{i,j,k,m} &:= \langle\varphi_i \otimes \varphi_j \mid V\varphi_k \otimes \varphi_m\rangle \\ c_i^* &:= c^*(\varphi_i) \quad , c_j := c(\varphi_j). \end{aligned}$$

We define the Hartree-Fock (HF) energy

$$E_{\mathrm{hf}}(N) := \inf\left\{\langle\Phi|H\Phi\rangle|\Phi \in \mathcal{SD}_N\right\}$$

to be the infimum over all Slater determinants of the expectation value of the considered Hamiltonian (A.2)*, where by Slater determinant we mean an element of the set*

$$\mathcal{SD}_N := \left\{\Phi = \prod_{n=1}^{N} c^*(\varphi_n)\Omega \in \mathcal{F}(\mathfrak{H}) \mid \exists\varphi_1, \ldots, \varphi_N : \langle\varphi_n|\varphi_m\rangle = \delta_{n,m}\right\},$$

of all normalized vectors represented as an anti-symmetrized tensor product.

Remark A.1. In the case of a Slater determinant $\Phi \in \mathcal{SD}_{\mathcal{N}}$ we can characterize the 1-pdm by projections and the 2-pdm by the 1-pdm as in Lemma A.1. Therefore the HF energy can be written as follows:

$$\begin{aligned}
E_{\mathrm{hf}}(N) &= \inf\left\{\mathrm{Tr}_{\mathfrak{H}}\left[h\gamma^1_\Phi\right] + \frac{1}{2}\mathrm{Tr}_{\mathfrak{H}\times\mathfrak{H}}\left[V\gamma^2_\Phi\right] \mid \Phi \in \mathcal{SD}_{\mathcal{N}}\right\} \\
&= \inf\left\{\mathrm{Tr}_{\mathfrak{H}}\left[h\,\gamma^1_\Phi\right] + \frac{1}{2}\mathrm{Tr}_{\mathfrak{H}\times\mathfrak{H}}\left[V(1-\mathrm{Ex})(\gamma^1_\Phi \otimes \gamma^1_\Phi)\right] \mid \Phi \in \mathcal{SD}_{\mathcal{N}}\right\} \\
&=: \inf\left\{\mathcal{E}_{\mathrm{hf}}(\gamma) \mid \gamma = \gamma^* = \gamma^2, \mathrm{Tr}_{\mathfrak{H}}(\gamma) = N\right\}.
\end{aligned}$$

Appendix B

Riesz Projection

Lemma B.1. *Let $n \in \mathbb{N}$, $A \in M^{\mathbb{C}}_{n\times n}$, $N \in \mathbb{N}$, and $\lambda_1, \lambda_2, \ldots, \lambda_N$ be the nonzero, not real, pairwise distinct eigenvalues of A with multiplicity $n_1, \ldots, n_N$. Then*

$$\mathbb{1}\left[A<0\right] = \frac{-1}{2\pi i}\int\limits_{\mathbb{R}} (A - zI)^{-1} dz - \frac{1}{2} I. \tag{B.1}$$

Proof. In [23] it was proven that every projection onto the eigenvalues of A can be written in the form

$$P_j = \frac{-1}{2\pi i}\oint\limits_{\Gamma_R} (A - zI)^{-1} dz, \tag{B.2}$$

where Γ_R is a smooth closed curve in $\mathbb{C}$ which contains all points z with $|z - \lambda_j| = R$, where

$$0 < R < \min\left\{|\lambda_j - \lambda_k| \mid j, k \in \{1, \ldots, N\}, j \neq k\right\}. \tag{B.3}$$

It remains to show that

$$\lim_{R\to\infty} \frac{-1}{2\pi i}\oint\limits_{\Gamma_R} (A - zI)^{-1}\, dz = \frac{-1}{2\pi i}\int\limits_{\mathbb{R}} (A - zI)^{-1} dz - \frac{1}{2} I. \tag{B.4}$$

In the following we need line integrals of the form

$$\int\limits_K R(A, z)\, dz, \tag{B.5}$$

with curves K in the resolvent set $\rho(A)$. These integrals are defined componentwise as follows:
Let $G \subseteq \mathbb{C}$ be an open subset, $K \subseteq G$ be a curve in G. Moreover let

$$A(.) : G \longrightarrow M_{n\times n}(\mathbb{C})$$

be a holomorphic mapping for each $n \in \mathbb{N}$. Then

$$\int_K A(z)dz := \begin{pmatrix} \int_K a_{11}(z)dz & \dots & \int_K a_{1n}(z)dz \\ \vdots & \vdots & \vdots \\ \int_K a_{n1}(z)dz & \dots & \int_K a_{nn}(z)dz \end{pmatrix}. \tag{B.6}$$

Furthermore, if $w = (w_1, \dots, w_n) \in \mathbb{C}^n$, then we have

$$\begin{aligned} \int_K A(z)wdz &:= \int_K \left(\sum_{j=1}^n a_{1j}(z)w_j, \dots, \sum_{j=1}^n a_{nj}(z)w_j \right) dz \\ &:= \left(\int_K \sum_{j=1}^n a_{1j}(z)w_j dz, \dots, \int_K \sum_{j=1}^n a_{nj}(z)w_j dz \right). \end{aligned} \tag{B.7}$$

For $A \in M_{n\times n}(\mathbb{C})$ we remark that $R(A,z) = (A - zI)^{-1}$ is holomorphic for every $z \in \rho(A)$, where

$$\rho(A) = \mathbb{C} \setminus \{\lambda \mid \lambda \in \mathbb{C}, \lambda \text{ eigenvalue of } A\}, \tag{B.8}$$

i.e., all $\mathbb{C}$ except finitely many isolated points. Moreover for $z \in \rho(A)$ we define $(A - zI)^{-1}$ with the representation of the inverse matrices as follows

$$(A - zI)^{-1} = \frac{1}{\det(A - zI)} \begin{pmatrix} A_{11}(A - zI) & \dots & A_{n1}(A - zI) \\ \vdots & \vdots & \vdots \\ A_{n1}(A - zI) & \dots & A_{nn}(A - zI) \end{pmatrix}, \tag{B.9}$$

where $\det(A - zI)$ is a polynomial of degree n, its zeros are the eigenvalues of A and the cofactor matrices $A_{k,j}(A - zI)$ with $k, j \in \{1, 2, \dots, n\}$ are the determinant of the $(n-1) \times (n-1)$ matrices that results from deleting row k and column j of $A - zI$. For $z \in \rho(A)$ with $|z| \geq \|A\|_{\mathrm{op}}$ the Neumann series for $(A - zI)^{-1}$ is given by

$$(A - zI)^{-1} = -\frac{1}{z}(I - \frac{A}{z})^{-1} = -\frac{1}{z}\sum_{k=0}^{\infty}(\frac{A}{z})^k. \tag{B.10}$$

In particular

$$\left\|(A - zI)^{-1}\right\|_{op} \leq \frac{1}{|z|}\sum_{k=0}^{\infty}\left(\frac{\|A\|_{op}}{|z|}\right)^k = \frac{1}{|z|}\frac{1}{1 - \frac{\|A\|_{op}}{|z|}}. \tag{B.11}$$

We now consider the path $\Gamma_R = C_R + [-iR, iR]$, where C_R is a semicircle around zero with radius R large enough to enclose all the singular points of the integrand and remark for $0 \neq z \in \rho(A)$ that

$$\begin{aligned}(A - zI)^{-1} + \frac{1}{z}I &= (A - zI)^{-1}\left[I + \frac{1}{z}(A - zI)I\right] \\ &= \frac{1}{z}(A - zI)^{-1}A. \end{aligned} \tag{B.12}$$

Using polar coordinates $z = R\,e^{i\varphi}$ to compute the integral over the semicircle C_R we get

$$\begin{aligned} -\frac{1}{2\pi i}\int\limits_{C_R}(A - zI)^{-1}dz &= -\frac{1}{2\pi i}\left[\int\limits_{C_R}\frac{1}{z}Idz + \int\limits_{C_R}\frac{1}{z}(A - zI)^{-1}Adz\right] \\ &= -\frac{1}{2\pi i}\left[\int\limits_0^\pi \frac{1}{R}e^{-i\phi}IRie^{i\phi}d\phi + \int\limits_0^\pi \frac{1}{R}\,e^{-i\phi}\,(A - Re^{i\phi}I)^{-1}\,A\,R\,i\,e^{i\phi}\,d\phi\right] \\ &= -\frac{1}{2}I - \frac{1}{2\pi i}\int\limits_0^\pi \frac{1}{R}\,e^{-i\phi}\,(A - Re^{i\phi}I)^{-1}\,A\,R\,i\,e^{i\phi}\,d\phi, \end{aligned} \tag{B.13}$$

but the integrand $\frac{1}{R}\,e^{-i\phi}\,(A - Re^{i\phi}I)^{-1}\,A\,R\,i\,e^{i\phi}$ in operator norm tends to zero as R tends to ∞. Indeed,

$$\begin{aligned} \left\|\frac{1}{R}e^{-i\phi}(A - Re^{i\phi}I)^{-1}ARie^{i\phi}\right\|_{op} &\leq \left\|(A - Re^{i\phi}I)^{-1}\right\|_{op}\|A\|_{op} \\ &\leq \frac{1}{R}\,\frac{1}{1 - \frac{\|A\|_{op}}{R}}\;\|A\|_{op} \underset{R\to\infty}{\longrightarrow} 0. \end{aligned} \tag{B.14}$$

We now apply the following theorem

Theorem B.1. *Let $G \subseteq \mathbb{C}$ and $f \in C^0(G, \mathbb{C})$. Let moreover $\varphi(.) \in C^1([a,b], \mathbb{C})$ be a regular path in $\mathbb{C}$ with $Ran(\varphi(.)) \subseteq G$, which represents a curve $K : t \longmapsto \varphi(t)$ for $t \in [a,b]$. Then*

$$\left|\int\limits_K f(z)dz\right| \leq \int\limits_a^b |f(\varphi(t))|\,|\varphi'(t)|\,dt \leq \max_{t\in[a,b]} |f(\varphi(t))|\,|K|, \tag{B.15}$$

together with the estimate

$$\max_{k,j\in\{1,2,\ldots,n\}} |a_{kj}| \leq \|A\| \leq \left(\sum_{k,j=1}^n |a_{kj}|^2\right)^{\frac{1}{2}} \leq n \cdot \max_{k,j\in\{1,2,\ldots,n\}} |a_{kj}|, \tag{B.16}$$

and use (B.14) to get

$$\begin{aligned}\left|\int_{C_R} \frac{A}{z(A-zI)}dz\right| &\leq \int_0^\pi \frac{1}{R}e^{-i\phi}(A-Re^{i\phi}I)^{-1}ARie^{i\phi}d\phi \\ &\leq \max_{\phi\in[0,\pi]}\left|(A-Re^{i\phi}I)^{-1}A\right||C_R| \\ &\leq \left\|(A-Re^{i\phi}I)^{-1}A\right\|_{op}|C_R| \underset{R\to\infty}{\longrightarrow} 0. \end{aligned} \tag{B.17}$$

But this means that

$$\lim_{R\to\infty}\left\|\int_0^\pi \frac{1}{R}e^{-i\phi}(A-Re^{i\phi}I)^{-1}ARie^{i\phi}d\phi\right\|_{op} = 0. \tag{B.18}$$

□

Appendix C

Lattice in the d-Dimensional Euclidean Space $\mathbb{R}^d$

Definition C.1. *Let $x_1, x_2, \ldots, x_d$ be linearly independent vectors in a $d-$dimensional Euclidean space. The set of all vectors*

$$\Gamma = \left\{ x \in \mathbb{R}^d \mid x = \sum_{i=1}^{d} n_j x_j, n_j \in \mathbb{Z} \right\}, \tag{C.1}$$

where $\mathbb{Z}$ is the ring of integers, is called a lattice in $\mathbb{R}^d$. The vectors $\{x_j\}_{j=1}^{d}$ are called a basis for the lattice Γ.

A basis for the lattice can be chosen in various ways and two bases for a lattice are connected by a unimodular integral matrix. For any two lattices Γ_1 and Γ_2 in $\mathbb{R}^d$ there is a non-singular transformation a such as $\Gamma_1 = a\Gamma_2$. In particular, any lattice in $\mathbb{R}^3$ is an affine image of the cubic lattice $\mathbb{Z}^d$ consisting of all vectors with integer coordinates in some fixed orthonormal basis in $\mathbb{R}^d$.

Definition C.2. *The lattice Γ' which consists of all vectors x' such that the inner product $\langle x \mid x' \rangle$ is an integer for all $x \in \Gamma$ is called the reciprocal lattice to Γ.*

According to this definition we can introduce the dual lattice Γ^* to a given lattice Γ by

$$\Gamma^* = 2\pi\Gamma', \tag{C.2}$$

where multiplication of a lattice by a number (in this case 2π) means that all the vectors of the lattice are multiplied by this number. The normalization in (C.2) turns out to be convenient in the theory of periodic operators.

C.0.5 Fundamental Sets and Fundamental Regions of a Lattice

Two points $x, y \in \mathbb{R}^d$ are said to be congruent mod Γ if $x - y \in \Gamma$. This is written $x \equiv y \bmod \Gamma$. Congruence mod Γ determines an equivalence relation on the point set $\mathbb{R}^d$. The quotient set $\mathbb{R}^d/\Gamma := F$ is called a fundamental set (FS) of the lattice Γ. The FS F can be chosen as a subset of $\mathbb{R}^d$ in various ways. However, it is always assumed that F is a measurable set. The Lebesgue measure of F is denoted by τ and does not depend on the specific choice of F. We have the relations $\tau\tau' = 1$ and $\tau = \tau^* = (2\pi)^d$, where τ' and τ^* are the Lebesgue measures of F' and F^* respectively.

Lemma C.1. *The following statements are equivalent:*

1. *F is a fundamental set of the lattice Γ.*
2. *F is measurable and the translates $\{xF\}_{x\in\Gamma}$ cover all of $\mathbb{R}^d$ with multiplicity one, i.e., $\bigcup\limits_{x\in\Gamma} \{xF\} = \mathbb{R}^d$ and $x_1F \cap x_2F = \emptyset$ for $x_1 \neq x_2$.*
3. *F is measurable and for any translation $k \in \mathbb{R}^d$, the set kF contains precisely one point of Γ.*

A fundamental set is obviously neither open nor closed. Therefore, it is sometimes more convenient to work with a fundamental region (FR) of F, which is defined as an open set $\mathcal{F}$ such that for some FS F

$$\mathcal{F} \subset F \subset \mathcal{F} \cup \partial\mathcal{F},$$

where $\partial\mathcal{F}$ is the boundary of $\mathcal{F}$. For example the Dirichlet-Voronoi-parallelohedron

$$M := \{k : |k| < |k - x|\,, x \in \Gamma \setminus \{0\}\}\,.$$

represents the points k which are closer to the origin than to any other point of Γ. In solid state physics the set M is known as the first Brillouin zone. If $\mathcal{F}$ is a given FR of a lattice, then it is always possible to obtain FS F from it. It suffices to adjoin to $\mathcal{F}$ a part of $\partial\mathcal{F}$ that is the quotient set $\partial\mathcal{F}/\Gamma$. The following assertion follows from Lemma C.1.

Lemma C.2. *An open set $\mathcal{F}$ is a fundamental region of a lattice Γ if and only if*

1. *no two points of $\mathcal{F}$ are congruent modulo Γ.*
2. *$\forall k \in \mathbb{R}^d$, $\exists k_1 \in \mathcal{F} \cup \partial\mathcal{F}$ such that $k \equiv k_1$ mod Γ.*

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